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## Open quantum systems in and out of equilibrium: theory and applications

## Andreu Riera-Campeny

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# Open quantum systems in and out of equilibrium <br> <br> theory and applications 

 <br> <br> theory and applications}

by<br>Andreu Riera-Campeny<br>under the supervision of<br>Prof. Anna Sanpera Trigueros<br>and<br>PhD. Philipp Strasberg

A thesis submitted in partial fulfillment for the degree of Doctor of Philosophy in Physics

Física Teòrica: Informació i Fenòmens Quàntics<br>Departament de Física, Facultat de Ciències



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A la gent que estimo.

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## Abstract

Quantum mechanics is the physical theory that governs the behavior of atomic and subatomic particles, as well as their interactions. The behavior of physical systems at those tiny scales challenges our intuition, which is build upon our daily experience. The reason why quantum properties, like quantum coherence, entanglement, or non-locality, do not survive in the macroscopic scale is still open to discussion. Part of the answer resides on the fact that, at a practical level, all quantum systems interact with their environment. They are open quantum systems. Although the interaction with the environment is in practice unavoidable, it is not necessarily detrimental. In fact, the open system dynamics is crucial for many applications, including cooling, particle or energy transport, or information processing.

Open quantum systems are often considered to be in contact with an infinite environment at equilibrium, which makes the problem more tractable at a theoretical level. While this idealization has lead to a plethora of results, for instance, in quantum optical platforms, it also imposes strong assumptions on the dynamics that are not always satisfied. If the assumption of the infinite environment at equilibrium is relaxed, describing the dynamics of open quantum systems becomes more challenging, in particular when the environment develops nonequilibrium features during the evolution, or when memory effects cannot be disregarded.

In this thesis, we develop a weak-coupling master equation approach to tackle the nonequilibrium dynamics of open quantum systems in contact with finite environments. To this end, we include in the description a dynamically evolving environment and keep track, at a coarse-grained level, of the system environment correlations. We complement this dynamical description with a thermodynamic framework, from which the first and second law of thermodynamics are found as a consequence of the underlying microscopic description.

We also explore the dynamics of open quantum systems beyond the weakcoupling limit, taking advantage of more standard approaches like the formalism of quantum operations, or the quantum Langevin equation. While these techniques have been studied in the literature, we use them to tackle new problems involving exotic phases of matter or asymmetric heat transport.

## Resum

La mecànica quàntica és la teoria que governa el comportament de les partícules atòmiques i subatòmiques, així com les seves interaccions. El comportament dels sistemes físics a aquestes escales diminutes desafien la nostra intuïció, que està basada en la nostra experiència diària. La raó per la qual les propietats quàntiques, com la coherència quàntica, l'entrellaçament o la no localitat, no sobreviuen a l'escala macroscòpica està encara oberta a debat. Part de la resposta rau en el fet que, en l'àmbit pràctic, tots els sistemes quàntics interaccionen amb el seu entorn. Són sistemes quàntics oberts. Tot i que la interacció amb l'entorn és inevitable, no és necessàriament perjudicial. De fet, la dinàmica de sistemes oberts és crucial per moltes aplicacions, per exemple, el refredament, el transport de partícules o energia, o el processament d'informació.

Els sistemes quàntics oberts sovint es consideren en contacte amb un entorn infinit i en equilibri, fet que torna el problema més tractable en l'àmbit teòric. Tot i que aquesta idealització ha portat a una plètora de resultats, per exemple, en plataformes d'òptica quàntica, també imposa hipòtesis restrictives a la dinàmica que no sempre es compleixen. Si relaxem la hipòtesi d'un entorn infinit, la descripció de la dinàmica dels sistemes quàntics oberts es torna més exigent, en particular quan l'entorn desenvolupa trets de no equilibri durant l'evolució, o quan els efectes de memòria no es poden obviar.

En aquesta tesi, desenvolupem una equació mestra d'interacció dèbil per descriure la dinàmica de no equilibri de sistemes quàntics oberts que estan en contacte amb un entorn finit. Amb aquesta finalitat, incloem en la descripció un entorn que evoluciona de manera dinàmica i fem un seguiment, a nivell aproximat, de les correlacions entre el sistema i l'entorn. Complementem aquesta descripció dinàmica amb un marc termodinàmic, a partir del qual la primera i segona llei de la
termodinàmica sorgeixen a conseqüència de la descripció microscòpica subjacent.
A més, també explorem la dinàmica de sistemes quàntics oberts més enllà del límit d'interacció dèbil, aprofitant tècniques més estàndard com el formalisme d'operacions quàntiques o l'equació de Langevin quàntica. Tot i que aquestes tècniques han sigut estudiades anteriorment en la literatura, les utilitzem per atacar problemes nous que tenen a veure amb estats exòtics de la matèria o el transport de calor asimètric.

## Resumen

La mecánica cuántica es la teoría que gobierna el comportamiento de las partículas atómicas y subatómicas, así como sus interacciones. El comportamiento de los sistemas físicos a estas escalas diminutas desafían nuestra intuición, que está basada en nuestra experiencia diaria. La razón por la que las propiedades cuánticas, como la coherencia cuántica, el entrelazamiento o la no localidad, no sobreviven a la escala macroscópica está todavía abierta a debate. Parte de la respuesta radica en el hecho de que, en el ámbito práctico, todos los sistemas cuánticos interaccionan con su entorno. Son sistemas cuánticos abiertos. Aunque la interacción con el entorno es inevitable, no es necesariamente perjudicial. De hecho, la dinámica de sistemas abiertos es crucial para muchas aplicaciones, por ejemplo, el enfriamiento, el transporte de partículas o energía, o el procesamiento de información.

Los sistemas cuánticos abiertos a menudo se consideran en contacto con un entorno infinito y en equilibrio, lo que vuelve el problema más tratable en el ámbito teórico. Aunque esta idealización ha llevado a una plétora de resultados, por ejemplo, en plataformas de óptica cuántica, también impone hipótesis restrictivas a la dinámica que no siempre se cumplen. Si relajamos la hipótesis de un entorno infinito, la descripción de la dinámica de los sistemas cuánticos abiertos se vuelve más exigente, en particular cuando el entorno desarrolla rasgos de no equilibrio durante la evolución, o cuando los efectos de memoria no se pueden obviar.

En esta tesis, desarrollamos una ecuación maestra de interacción débil para describir la dinámica de no equilibrio de sistemas cuánticos abiertos que están en contacto con un entorno finito. Con este fin, incluimos en la descripción un entorno que evoluciona de manera dinámica y hacemos un seguimiento, a nivel aproximado, de las correlaciones entre el sistema y el entorno. Complementamos esta descripción dinámica con un marco termodinámico, a partir del cual la primera
y segunda ley de la termodinámica surgen como consecuencia de la descripción microscópica subyacente.

Además, también exploramos la dinámica de sistemas cuánticos abiertos más allá del límite de interacción débil, aprovechando técnicas más estándar como el formalismo de operaciones cuánticas o la ecuación de Langevin cuántica. Aunque estas técnicas han sido estudiadas anteriormente en la literatura, las utilizamos para atacar problemas nuevos que tienen que ver con los estados exóticos de la materia o el transporte de calor asimétrico.

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## Declaration

I declare that the thesis has been composed by myself and that the work has not been submitted for any other degree or professional qualification. I confirm that the work submitted is my own, except where work which has formed part of jointly-authored publications has been included. My contribution and those of the other authors to this work have been explicitly indicated below. I confirm that appropriate credit has been given within this thesis where reference has been made to the work of others.

## List of Publications

[RMP+19] A. Riera-Campeny, M. Mehboudi, M. Pons, and A. Sanpera, "Dynamically induced heat rectification in quantum systems", Phys. Rev. E 99, 032126 (2019).
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## About this thesis

This thesis contains most of the research I have carried in the field of open quantum systems at the Quantum Information Group (GIQ) at the Autonomous University of Barcelona, from October 2017 to October 2021 under the supervision of Anna Sanpera and Philipp Strasberg.

From describing the interaction of a single hydrogen atom with the electromagnetic background to understanding the Hawking radiation that comes out of a black hole, the theory of open quantum systems has found applications in very diverse branches of physics. This thesis aims at giving a self-contained but not complete picture of the theory of open quantum systems from my personal point of view. Chapters 1 and 2 briefly review part of the literature in open quantum systems and motivate the open questions that we discuss in this thesis. Chapters 3 and 4 are the theory core of this thesis, and discuss the dynamic and thermodynamic implications of open systems that interact with finite environments. Chapters 6 and 5 move beyond the master equation paradigm, and study applications of previously developed theory. Finally, the conclusions are presented in Chap. 7.

My hope is that this thesis is sufficiently self-contained for non-experts in open quantum systems to follow the discussion and the derivations but, at the same time, readers with more expertise still can find it insightful and interesting (maybe skipping some parts). While I am not sure that this approach is of everyone's taste, I think that is what I would have liked to read when I started my PhD.

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At the beginning there was only Chaos.

- Aristophanes


## Introduction

Physics $\varphi$ v́бıऽ, (literally Nature) is the scientific discipline that studies all natural phenomena. Within physics, quantum mechanics is concerned about the behavior of atomic and subatomic particles and its interactions. The behavior at such small scales can differ significantly from that of our daily experience. For instance, exotic phenomena like quantum coherence, entanglement, or non-locality are exclusively observed at the microscale. The precise reason why the quantum behavior is not observed at the macroscale remains a matter of debate. However, it is known that part of the answer resides in the fact that, at a practical level, all quantum systems interact with their environment. They are open quantum systems.

Quantum features are often desired for practical applications. Since open quantum system dynamics are, in certain regimes, responsible for the loss of those quantum features, they are also known as noisy. However, this nomenclature has a bad connotation that is not always justified. While open system dynamics are sometimes responsible for decoherence, they also enable more general transformations between quantum states. For this reason, they are essential for certain applications like, for instance, cooling, particle transport, or information processing.

### 1.1 Background and context

The environment of an open quantum system often has many degrees of freedom and is uncontrollable. Thus, it is necessary to have effective descriptions of the dynamics of the open quantum system where only the relevant environment information is included. This is the case, for instance, of quantum master equations. Master equations have the advantage that they apply to a large class of open systems, are intuitive, and often allow further analytical progress in the description.

Contrary to more modern applications, quantum master equations were introduced to study the dynamics of the energy populations of closed quantum systems. Their history starts in 1928, with a seminal work of Pauli [Pau28]. There, he presented a master equation for the evolution of the energy populations of a weakly perturbed closed system using the random phase approximation. His master equation took the simple form of a probability balance equation, which nowadays is often referred to as the Pauli master equation. Strictly speaking, Einstein already used a master equation to describe the quantum theory of radiation in [Ein17] ten years before Pauli. However, Einsteins' master equation description was based on purely statistical arguments, while Pauli derived it from an underlying microscopic description.

In 1953, a similar quantum master equation approach was used by Wangsness and Bloch to study the dynamics of nuclear spin populations [WB53]. Interestingly, Wangsness and Bloch already used the idea of a system interacting with an environment that was in a diagonal state in the energy eigenbasis. Similar ideas also appeared in related studies of angular momentum and spin relaxation around that time [AP53; Sol55]. In 1957, Redfield improved the theory of Wangsness and Bloch, obtaining the first approximated master equation that also included the dynamics of the off-diagonal elements of the density matrix [Red57]. Even though the equation was derived in the context of nuclear magnetic resonance, Redfield already acknowledged that it could be applied to more general problems, like Brownian motion or spin dynamics. That quantum master equation, known as the Redfield equation, is still used today.

Master equations were also used to study how the macroscopic irreversibility arises from the underlying reversible dynamical laws. After the works of Onsager [Ons31a; Ons31b] in 1931, irreversible equilibration processes were understood in terms of first-order differential equations that fulfilled certain symmetry relations that became known as the Onsager relations. In 1954, an enlightening work from van Kampen [Van54] used the master equation approach of Pauli [Pau28] together with a coarse graining procedure inspired by von Neumann [Neu29] (see
[Neu10] for the English translation) to derive from a microscopic description the phenomenological equations of Onsager as well as their symmetry relations.

During the decades of 1950s and 1960s, quantum master equations were gathering popularity. Motivated by understanding the dynamics of the energy populations in the problem posed by Pauli, a series of papers derived four types of generalized (or exact) quantum master equations. The first of those exact master equations was obtained by van Hove [Van57] and later generalized by Swenson [Swe62]. The second type was obtained by Nakajima [Nak58] and independently and in greater detail by Zwanzig [Zwa60; Zwa61]. The third type was obtained first by Résibois [Rés61] and shortly after modified by Prigonie and Résibois [PR61]. The fourth type was derived by Montroll [Mon62]. Despite the fact that all the equations were exact, it was not known whether they were equivalent. It was not until later works from Résibois [Rés63] and Zwanzig [Zwa64], that it could be proven that the equations obtained by Nakajima and Zwanzig, Prigonie and Résibois, and Montroll where equivalent but not identical to the ones from van Hove and Swenson. Interestingly, the Pauli master equation is found as a special case of those generalized master equations.

Theoretically, the importance of exact master equations is that they provide the most general form of open quantum system evolutions. Nonetheless, because they are so general, they are also virtually impossible to solve in most of the situations. Hence, from the practical point of view, exact master equations are important because they provide a starting point to develop controlled approximated schemes. Then, the chosen approximation scheme as well as its range of validity depends on the particular problem to which the quantum master equation is applied. For instance, the Pauli master equation arises as a lower order expansion of a weakly-perturbed many-body system [Van57], and the Bloch equations arise in the limit of linear response of a nuclear spin interacting with a heat bath environment [AK64]. Other different approximation schemes were used to tackle the physics of irreversible dynamics in fields including superradiance, superconductivity, or the criticality of magnetism to name a few; see for instance, [Aga73; Haa73].

The derivation of a plethora of rigorous analytic results about open quantum systems triggered by the use of exact master equations also gathered the attention of the mathematical physics' community. In the decade of the 1970s, many results were derived in the context of dynamical semigroups. Those dynamical semigroups correspond to the family of evolution maps associated with a memoryless quantum evolution, and arise after certain simplifications of the exact master equations. A review of these results can be found in a number of publications; see for instance
[Aga73; Dav76; Ali79]. Of particular importance are the independent works of Gorini, Kossakowski, Sudarshan [GKS76] and Lindblad [Lin76], which provided the form of the most general generator of dynamical semigroups. Those two works established a deep connection between weak-coupling master equations and dynamical semigroups, thus providing quantum master equations with a solid mathematical background.

Of course, quantum master equations are not the only approach to investigate the dynamics of open quantum systems. An alternative technique is using the formalism of quantum operations (also quantum evolutions, or quantum channels), to describe the transformations that a state can undergo in the presence of the environment. This approach was put forward by Sudarshan, Mathews, and Rau in Ref. [SMR61]. The basic idea is to consider the most general transformation between quantum states and then impose restrictions that guarantee, roughly speaking, that the output of quantum operation is a quantum state if the input was a quantum state. This approach was refined in the successive years by a number of important results, from which we highlight the Kraus decomposition [Kra71], and the Jamiołkowski-Choi isomorphism [Jam72; Cho75]. While this approach is very useful and often even insightful in low dimensions, its complexity grows very quickly. For instance, for a Hilbert space of $N$ spin- $1 / 2$ particles, the most general quantum operation has $\left(2^{N}\right)^{4}$ elements.

Another possibility that has been extensively used in the literature is the socalled quantum Langevin equation. This approach was motivated by Ford, Kac, and Mazur in Ref. [FKM65] as a technique to study the equilibration dynamics of a Brownian particle. Analogously to the classical case, the quantum Langevin equation describes the evolution of the position of a quantum particle subject to friction and noise. The difference between the classical and the quantum equation is that the friction and noise have a quantum mechanical origin. To derive it, the authors assume that the Brownian particle interacts linearly with a collection of harmonic oscillators initially found in a thermal state. Then, it is possible to write down the expression for the friction and noise terms as a function of the oscillators' parameters as well as their initial temperature. Interestingly, the quantum Langevin equation admits an analytic solution if the Brownian particle happens to be also harmonically trapped.

Even though the quantum Langevin equation is obtained assuming a bath of harmonic oscillators, it can be phenomenologically applied to more general environments. In particular, if the equations of motion of the environment can be linearized around a certain equilibrium point, the quantum Langevin equation can still apply provided that the influence of the system on the environment is small.

However, it turns out that the resulting equation, unlike the classical case, becomes model dependent [CWL85]. Luckily, this problem disappears when the bath can be treated classically, even if the system preserves its quantum mechanical treatment.

Finally, we list for completeness other commonly used methods that we do not discuss here. Those are the Feynman-Vernon influence functional [FV63], Heisenberg picture methods [AKE73; KM75] and the input-output formalism [Yur84; GC85], the hierarchy of the equations of motion [TK89], the stochastic Schrödinger equation [Car93], and the process tensor [Lin79; MM21]. We also invite the interested reader to find more information in the excellent books and reviews [GZ00; BP02; Wei12; RH12; Sch14; VA17; Str21].

### 1.2 Narrowing the focus: the problem at hand

Describing open quantum systems far from equilibrium is challenging, in particular when the environment is mesoscopic (that is, large but not infinite), when it develops nonequilibrium features during the evolution, or when memory effects and systembath correlations cannot be fully disregarded.

In recent years, the miniaturization of quantum experiments towards the microscopic scale has led also to a more detailed description of their surroundings. As a consequence, one has access to some dynamical information about the environment, which could be potentially used to obtain more accurate predictions about the open quantum system dynamics in the aforementioned challenging scenarios. Then, it is timely to investigate how quantum master equations can profit from this extra information by including, to some extent, a dynamically evolving environment.

Including more dynamical information comes, however, at a price. One could be tempted to include as much information as possible from the environment, having the impression that this would always lead to more accurate predictions. But of course, this strategy requires humongous computational resources even for relatively small environments of, say, a hundred particles. On the other end of the spectrum, including no dynamical information about the environment often leads to an oversimplified description that may have no predictive power. Hence, the task of the physicist is to identify which and when are those relevant dynamical variables worth including in the description.

Which? Identifying the set of relevant variables is not an unfamiliar task in physics. Disciplines like classical statistical mechanics have to deal with this situation all the time. For instance, in many situations, an ideal gas of $10^{23}$ particles is well characterized by only, say, its volume, its pressure, its temperature, and its number of particles. In the microscopic scale, however, those relevant variables can
be less easily related to macroscopic features. In classical or quantum mechanics, the dynamics of a particle is generated by its energy operator (or Hamiltonian). Hence, it comes as no surprise that energy is always closely related to the microscopic relevant variables. For instance, the average energy of the environment or the probability to find a certain energy after a measurement are, in the certain regimes, examples of relevant dynamical variables at the microscale.

When? Understanding when it is important to consider some environment property as a dynamical variable is not an easy task. As a rule of thumb, the larger the size of the environment, the less important it is to consider its properties as dynamical variables. The intuition is as follows. If both the open quantum system and the environment contain a single particle, the state of one becomes very much dependent on the state of the other. In other words, the state of the open quantum system influences the environment and also the other way around. However, if suddenly the environment contains thousands of particles, the dynamics of the open system is only affected by certain global properties of the environment, upon whose dynamics has only little effect. In the limit in which this effect can be neglected, one can consider that global property to be found in a given reference state without need of finding how it evolves. Hence, it is no longer a relevant dynamical variable.

Given the lack of master equation approaches that make use of dynamical environment information, in this thesis, we aim at providing a self-contained master equation approach to study the dynamics of open quantum systems that interact with dynamically evolving environments. To that end, we use the NakajimaZwanzig exact master equation as a starting point to derive a perturbative approximation scheme for weak system-environment interactions. Since our approach includes dynamical bath information, we are able to extend the range of validity of weak-coupling quantum master equations beyond the paradigm of an infinite, steady, and memoryless environment. Equipped with this technique, we aim at answering the following theoretical questions:
(TQ1) What does our approach reveal about open quantum system dynamics?
(TQ2) How does our approach connect to previously used techniques?
(TQ3) Is it possible to complement our approach with a nonequilibrium thermodynamic framework?
(TQ4) What does this new thermodynamic framework reveal?
So far, our focus has been on deriving new theory that takes advantage of the bath dynamical information. In the second part of the thesis, we focus on
more practical applications that exploit already existing techniques to tackle the dynamics of open quantum systems.

The first and second practical questions are related to understanding which knowledge can be extracted from the spectral properties of a certain quantum evolution by using the formalism of quantum operations. In particular, we want to exploit the fact that the spectrum of a valid quantum evolution lies within the unit disk to understand the limitations of such quantum operations. We aim at answering the first and second practical questions:
(PQ1) Can the spectral properties of a quantum evolution give information about (dynamical) phases of matter?
(PQ2) Which is the general form of a quantum evolution (operation) that leaves invariant a collection of pure states?

The third practical question is related to heat transport through a collection of harmonic oscillators (the harmonic network). Given a harmonic network which is in contact with two heat baths at different temperatures, it is known that the stationary heat current flowing through the system is symmetric; that is, if one reverses the temperature bias, the heat current picks up a minus sign. While the asymmetric heat conduction is desirable for some applications, it has only been achieved using nonlinear interactions which are not present in the harmonic network. Hence, we want to answer to the third practical question:
(PQ3) Is it possible to achieve asymmetric heat transport through a harmonic network?
which we try to answer using the quantum Langevin equation approach.
We shall return to the theoretical questions (TQ1)-(TQ4) and the practical questions (PQ1)-(PQ3) at the conclusions' chapter.

### 1.3 Structure of the thesis

In the following, we summarize our main results, which also serves as an outline for the rest of the thesis.

In Chap. 2, we start introducing the basic notions of quantum mechanics and introduce the notation that we will use in the rest of the thesis. Then, we present a self-contained derivation of the Pauli, Redfield and Born-Markov-secular master equations in the weak-coupling limit, as methods to approach the dynamics of open quantum systems. Afterwards, we introduce the Nakajima-Zwanzig theory
and show that the aforementioned master equations can be obtained as particular applications of this theory. We conclude by connecting the open quantum system dynamics with the standard definitions of work, entropy and heat in quantum thermodynamics.

In Chap. 3, we discuss how to approach the dynamics of open quantum systems that are in contact with a finite bath, which is one of the central topics of this thesis. We derive the extended microcanonical master equation, study its properties, and apply it to a particular model in which we can benchmark against the exact dynamics. Also, we study how to recover the Born-Markov-secular master equation from our approach, which leads to a definition of a nonequilibrium effective temperature. This procedure leads to a hierarchy of master equations, in which each master equation gives more accurate predictions by using more dynamical information about the bath.

Chapter 4 is devoted to understand the dynamics of the extended microcanonical master equation from a thermodynamic point of view. In particular, we give meaningful definitions of internal energy, work, heat, and entropy, which we later use in order to derive the first and second law of thermodynamics, as well as the Clausius inequality. Then, we study the implications of Clausius inequality for finite baths, which reveals that universal reduction of the entropy production of nanoscale devices.

We dedicate Chap. 5 we move beyonnd weak-coupling master equations and study the spectral properties of general quantum evolutions. In particular, we are interested in proving that the spectrum of valid quantum evolutions lies within the unit disk. Then, we apply this spectral knowledge to two problems. The first is to identify a dynamical phase of matter known as the discrete time crystal. The second is to characterize the most general map that has as many fixed points as the dimension of the space.

In Chap. 6 we introduce the quantum Langevin equation approach to study the stationary dynamics of harmonic systems with and without periodic driving. Then, we move forward to investigate whether such periodic driving can be exploited to obtain asymmetric heat transport in harmonic systems.

Finally, we present an outlook of the thesis and our conclusions in Chap. 7.

## 2

## Preliminaries

This chapter sets up the stage to understand the theory of open quantum systems that follows in the upcoming chapters. In particular, we slowly introduce the basic concepts and tools, which hopefully help to fix the notation as well as establish the basic notions that will become relevant later. Then, we move to study the open quantum system dynamics and introduce the Pauli, Redfield and the Born-Markov-secular weak-coupling master equations. Afterwards, we introduce the Nakajima-Zwanzig theory, and see that all those master equations become particular applications of the theory. Finally, we introduce the "standard" framework of quantum thermodynamics from a dynamical viewpoint.

### 2.1 Notation and basic quantum mechanics

In quantum mechanics, one associates to every physical system a Hilbert space $\mathcal{H}$. The elementary elements of the Hilbert space are known as kets, and we represent them as $|\psi\rangle \in \mathcal{H}$. The dual element of a ket is a $\operatorname{bra}\langle\phi| \in \mathcal{H}^{*}$, and their inner product or braket is a scalar

$$
\begin{equation*}
\langle\phi \mid \psi\rangle \in \mathbb{C} . \tag{2.1}
\end{equation*}
$$

We say that $|\psi\rangle$ is normalized (or also is a pure state) if the inner product with itself is one $\langle\psi \mid \psi\rangle=1$. Instead, their outer product or ketbra is a linear operator

$$
\begin{equation*}
|\phi \times \psi| \in \mathrm{Op}(\mathcal{H}) \tag{2.2}
\end{equation*}
$$

which acts onto states as $(|\phi X \psi|)\left|\phi^{\prime}\right\rangle=\left\langle\psi \mid \phi^{\prime}\right\rangle|\phi\rangle$.

### 2.1.1 Quantum states

The state of a physical system is encoded into the density matrix $\rho \in \operatorname{Op}(\mathcal{H})$, which is nonnegative $\rho \geq 0$ and has trace one $\operatorname{tr}(\rho)=1$. Let $\{|i\rangle\}$ be an orthonormal basis of $\mathcal{H}$, then one can always expand

$$
\begin{equation*}
\rho=\sum_{i j} \rho_{i j}|i \chi j|, \tag{2.3}
\end{equation*}
$$

where $\rho_{i j}=\langle i| \rho|j\rangle$ are the density matrix components in the basis $\{|i\rangle\}$. Since quantum states are positive, they always admit a spectral decomposition; that is, it exists an orthonormal basis $\left\{\left|r_{i}\right\rangle\right\}$ of $\mathcal{H}$ such that

$$
\begin{equation*}
\rho=\sum_{i} r_{i}\left|r_{i} \times r_{i}\right| \quad \text { with } \quad r_{i} \in \mathbb{R} \tag{2.4}
\end{equation*}
$$

where $i=1, \cdots, d$ where $d$ is the dimension of the Hilbert space. The collection of eigenvalues $r_{i}$ is known as the spectrum of $\rho$, while $\left|r_{i}\right\rangle$ are the corresponding eigenvectors. Because $\rho$ is positive and has trace one, we find that $0 \leq r_{i} \leq 1$ and $\sum_{i} r_{i}=1$. That is, $\left\{r_{i}\right\}$ is a discrete probability distribution. From these properties, we observe that

$$
\begin{equation*}
\operatorname{tr}\left(\rho^{2}\right)=\sum_{i} r_{i}^{2} \leq 1 \tag{2.5}
\end{equation*}
$$

The $\operatorname{tr}\left(\rho^{2}\right)$ is known as the purity of the quantum state. Pure states fulfill $\operatorname{tr}\left(\rho^{2}\right)=1$, and can be written in the simple form $\rho^{2}=|\psi\rangle \psi \mid$, where $|\psi\rangle$ is normalized. The least pure state; that is, with a smaller value of $\operatorname{tr}\left(\rho^{2}\right)$ corresponds to $\rho=1 / d$ and it is known as the maximally mixed state.

### 2.1.2 Quantum measurements

A projective measurement $\{x, \Pi(x)\}$ is a collection of different measurement outputs $x \in \mathbb{R}$ and eigenprojectors $\Pi(x) \in \mathrm{Op}(\mathcal{H})$. The eigenprojectors $\Pi(x)$ are mutually orthogonal and complete; that is, $\Pi(x) \Pi\left(x^{\prime}\right)=\delta_{x, x^{\prime}} \Pi(x)$ and $\sum_{x} \Pi(x)=1$. Then,
performing the measurement $\{x, \Pi(x)\}$ in a system found in the state $\rho$ yields the output $x$ with probability $p(x)=\operatorname{tr}[\Pi(x) \rho]$ and leaves the system in the postmeasurement state

$$
\begin{equation*}
\rho^{\prime}(x)=\frac{\Pi(x) \rho \Pi(x)}{p(x)} . \tag{2.6}
\end{equation*}
$$

From a measurement $\{x, \Pi(x)\}$, one can always construct an observable $X=$ $\sum_{x} x \Pi(x)$ whose expectation value is given by

$$
\begin{equation*}
\langle X\rangle:=\sum_{x} x p(x)=\operatorname{tr}(X \rho) . \tag{2.7}
\end{equation*}
$$

Projective measurements are not the most general measurements in quantum mechanics. The so-called positive operator-valued measures or POVMs can be regarded as generalized measurements, which include projectors as a particular case. A POVM $\{y, P(y)\}$ is a set of measurement outputs $y \in \mathbb{R}$ and a set of positive operators $P(y)=K(y)^{\dagger} K(y) \in \mathrm{Op}(\mathcal{H})$ which are complete; that is, $\sum_{y} P(y)=\mathbf{1}$, but not necessarily orthogonal. Performing a POVM measurement on a state $\rho$ yields the output $y$ with probability $p(y)=\operatorname{tr}[P(y) \rho]$ and leaves the system in the post-measurement state

$$
\begin{equation*}
\rho^{\prime}(y)=\frac{K(y) \rho K(y)^{\dagger}}{p(y)} . \tag{2.8}
\end{equation*}
$$

The expectation value of $Y=\sum_{y} y P(y)$ is also given by the equation

$$
\begin{equation*}
\langle Y\rangle:=\sum_{y} y p(y)=\operatorname{tr}(Y \rho) . \tag{2.9}
\end{equation*}
$$

However, $Y$ is not an observable in the usual sense, since $\{y\}$ are not its eigenvalues and $P(y)$ are not eigenprojectors.

### 2.1.3 Quantum evolution

The evolution of an isolated quantum system is generated by the Schrödinger or Liouville-von Neumann equation, which reads ( $\hbar=1$ )

$$
\begin{equation*}
\partial_{t} \rho(t)=-i[H, \rho(t)], \tag{2.10}
\end{equation*}
$$

where $H=H^{\dagger}$ is the energy operator (or Hamiltonian) associated to the microscopic description of the physical system, and $\rho(t)$ is the state of the system at time $t$. If it
can be understood from the context, we will not write the time argument of the state; namely, $\rho(t) \mapsto \rho$. The solution of the Liouville-von Neumann equation is

$$
\begin{equation*}
\rho(t)=\exp (-i H t) \rho(0) \exp (i H t) \tag{2.11}
\end{equation*}
$$

We note that under the unitary dynamics (2.11) the purity is preserved; that is, $\operatorname{tr}\left[\rho(t)^{2}\right]=\operatorname{tr}\left[\rho(0)^{2}\right]$ for all $t$.

If one defines $X(t):=\exp (i H t) X \exp (-i H t)$, one can use the cyclic property of the trace to obtain the equivalence $\langle X\rangle(t)=\operatorname{tr}[X(0) \rho(t)]=\operatorname{tr}[X(t) \rho(0)]$. Hence, there is an alternative way to obtain the time-dependence of an expectation value. These two alternative procedures are known as the Schrödinger (for evolving states) and Heisenberg (for evolving observables) picture. In the Heisenberg picture, observables evolve according to the Heisenberg equation

$$
\begin{equation*}
\partial_{t} X(t)=i[H, X(t)] \tag{2.12}
\end{equation*}
$$

From Eq. (2.12) we see that the Hamiltonian $H$ is a conserved quantity of the evolution and, in particular, that the average energy $\langle H\rangle$ is preserved.

Actually, there are infinite intermediate pictures in between the Schrödinger and the Heisenberg picture. If the Hamiltonian $H=H_{0}+\lambda V$, where $V$ is a certain interaction, it is common to define the interaction picture with respect to the bare Hamiltonian $H_{0}$ where, both, observables and states evolve in time. It is done according to $\tilde{\rho}(t)=\exp \left(i H_{0} t\right) \rho(0) \exp \left(-i H_{0} t\right)$ and the evolution equation corresponds to

$$
\begin{equation*}
\partial_{t} \tilde{\rho}(t)=-i[\tilde{V}(t), \tilde{\rho}(t)] \tag{2.13}
\end{equation*}
$$

### 2.1.4 Composite quantum systems

Consider a composite quantum system whose corresponding Hilbert space $\mathcal{H}$ has two subsystems, say A and B. Then, their Hilbert space forms a tensor structure $\mathcal{H}=\mathcal{H}_{\mathrm{A}} \otimes \mathcal{H}_{\mathrm{B}}$. Expectation values of composite observables are computed according to Eq. (2.7). Instead, consider the local observables $X_{A} \otimes \mathbf{1}_{\mathrm{B}}$ and $\mathbf{1}_{\mathrm{A}} \otimes Y_{\mathrm{B}}$. Their expectation values are computed

$$
\begin{align*}
& \operatorname{tr}\left[\left(X_{\mathrm{A}} \otimes \mathbf{1}_{\mathrm{B}}\right) \rho\right]=\operatorname{tr}_{\mathrm{A}}\left[X_{A} \operatorname{tr}_{\mathrm{B}}(\rho)\right]=: \operatorname{tr}_{\mathrm{A}}\left(X_{\mathrm{A}} \rho_{\mathrm{A}}\right),  \tag{2.14}\\
& \operatorname{tr}\left[\left(\mathbf{1}_{\mathrm{A}} \otimes Y_{\mathrm{B}}\right) \rho\right]=\operatorname{tr}_{\mathrm{B}}\left[\operatorname{tr}_{\mathrm{A}}(\rho) Y_{\mathrm{B}}\right]=: \operatorname{tr}_{\mathrm{B}}\left(Y_{\mathrm{B}} \rho_{\mathrm{B}}\right), \tag{2.15}
\end{align*}
$$

where we have defined the reduced states $\rho_{\mathrm{A}}=\operatorname{tr}_{\mathrm{B}}(\rho)$ and $\rho_{\mathrm{B}}=\operatorname{tr}_{\mathrm{A}}(\rho)$. Hence, the reduced states of a subsystem are enough to compute expectation values of local observables. For composite quantum systems, we adopt the convention of not writing the identity matrices; that is, $X_{\mathrm{A}} \otimes \mathbf{1}_{\mathrm{B}} \mapsto X_{\mathrm{A}}$ whenever it can be understood from the context.

### 2.1.5 Quantum maps

The last object we discuss are quantum maps, which are also known as quantum channels, superoperators, or simply maps. A map $\mathcal{M}: \operatorname{Op}(\mathcal{H}) \mapsto \mathrm{Op}(\mathcal{H})$ is a linear transformation between operators in a Hilbert space. Of special interest are the socalled completely-positive and trace-preserving (CPTP) maps, which map quantum states to quantum states. We say that a quantum map $\mathcal{M}$ is trace-preserving if $\operatorname{tr}\{\mathcal{M}[\rho]\}=\operatorname{tr}[\rho]$ for all $\rho \in \mathrm{Op}(\mathcal{H})$. We say that a map $\mathcal{M}$ is completely positive if for any ancillary Hilbert space $\mathcal{H}_{\mathrm{A}}$ and any $\rho \in \operatorname{Op}\left(\mathcal{H}_{\mathrm{A}} \otimes \mathcal{H}\right)$ the combination $\left(\mathcal{I}_{\mathrm{A}} \otimes \mathcal{M}\right)[\rho] \geq 0$ if $\rho \geq 0$, where $\mathcal{I}_{\mathrm{A}}$ is the identity map in the ancillary space. Clearly, complete positivity implies positivity; that is, $\mathcal{M}[\rho] \geq 0$ if $\rho \geq 0$.

An example of a CPTP map is the evolution map $\mathcal{E}(t)$, which maps a given initial state $\rho(0)$ to an evolved state $\rho(t)=\mathcal{E}(t)[\rho(0)]$. Since maps are linear transformations, they are fully specified by the algebraic representation

$$
\begin{equation*}
\left.\mathcal{M}[\circ]=\sum_{i j i^{\prime} j^{\prime}} \mathcal{M}_{i j i^{\prime} j^{\prime}}\left\langle i^{\prime}\right|| | j^{\prime}\right\rangle \mid i\langle j| . \tag{2.16}
\end{equation*}
$$

where $\circ$ is a placeholder and $M_{i j i^{\prime} j^{\prime}} \in \mathbb{C}$. The four-index object $\mathcal{M}_{i j i^{\prime} j^{\prime}}$ is known as a tetradic, and behaves almost like a matrix acting on "vectors", which correspond to elements of $\mathrm{Op}(\mathcal{H})$.

The statement "almost like a matrix" can be made precise through a method known as vectorization. Namely, there exists an isomorphism between density matrices $\rho \in \operatorname{Op}(\mathcal{H})$ and kets in a doubled Hilbert space $|\rho\rangle\rangle \in \mathcal{H} \otimes \mathcal{H}$; which takes the form

$$
\begin{equation*}
\left.\rho=\sum_{i j} \rho_{i j}|i \nmid j| \leftrightarrow|\rho\rangle\right\rangle=\sum_{i j} \rho_{i j}|i\rangle|j\rangle . \tag{2.17}
\end{equation*}
$$

While transforming operators in $\rho, \sigma \in \mathrm{Op}(\mathcal{H})$ to vectors $|\rho\rangle\rangle \in \mathcal{H} \otimes \mathcal{H}$, one has to transform accordingly their inner product $\langle\langle\sigma \mid \rho\rangle\rangle=\operatorname{tr}\left[\sigma^{\dagger} \rho\right]$; which is known as the Hilber-Schmidt product. Then, the basis $\{|\mu\rangle\rangle=|i\rangle|j\rangle\}$ corresponds to the canonical orthonormal basis of the double Hilbert space.

Then, a quantum map $\mathcal{M}$ takes the form of a standard matrix in the doubled Hilbert space

$$
\begin{equation*}
\left.\left.\mathcal{M}[\rho]=\sum_{i j i^{\prime} j^{\prime}} \mathcal{M}_{i j i^{\prime} j^{\prime}} \rho_{i^{\prime} j^{\prime} \mid}\left|i \chi_{j}\right| \leftrightarrow \mathcal{M}|\rho\rangle\right\rangle=\sum_{\mu} \mathcal{M}_{\mu v} \rho_{v}|\mu\rangle\right\rangle . \tag{2.18}
\end{equation*}
$$

It is not difficult to check that, with the prescribed isomorphism, given two operators $X, Y \in \mathrm{Op}(\mathcal{H})$ the product $X \rho Y$ transforms according to

$$
\begin{equation*}
\left.X \rho Y \leftrightarrow|X \rho Y\rangle\rangle=X \otimes Y^{t}|\rho\rangle\right\rangle . \tag{2.19}
\end{equation*}
$$

### 2.1.6 A useful identity

To conclude this very first section, we state a useful identity for the exponential of two arbitrary matrices $X$ and $Y$, that is often appears in the weakly perturbed systems studied below. Namely, we note that

$$
\begin{equation*}
e^{t X}=e^{t Y}+\int_{0}^{t} d t^{\prime} e^{\left(t-t^{\prime}\right) Y}(X-Y) e^{t^{\prime} X} \tag{2.20}
\end{equation*}
$$

Equation (2.20) is easily proven by left multiplication by $\exp (-t Y)$ and derivation with respect to $t$.

### 2.2 Quantum Master Equations

Quantum master equations are one of the central topics of this thesis. Historically, the name master equation was introduced by Nordsieck, Lamb, and Uhlenbeck in Ref. [NLU40]. It was coined to refer to the following: "When the probabilities of the elementary processes are known, one can write down a continuity equation for $W$ [denoting a set of probabilities], from which all other equations can be derived and which we will call therefore the master equation." With time, the meaning of master equation became mostly restricted to refer to equations of the form

$$
\begin{equation*}
\partial_{t} p\left(\varepsilon_{i}\right)=\sum_{j \neq i}[w(i \mid j) p(j)-w(j \mid i) p(i)], \tag{2.21}
\end{equation*}
$$

where $p(i)$ correspond to the probability of being in a certain state $i$, and $w(i \mid j)$ are the transition rates of going from the state $j$ to the state $i$.

In quantum mechanics, those probabilities correspond to the diagonal entries $p(i)=\rho_{i i}=\langle i| \rho|i\rangle$ of the density matrix $\rho$ in a certain basis of interest $\{|i\rangle\}$. A quantum master equation is then the evolution equation of, not only the diagonal entries of the density matrix, but also of its coherences $\rho_{i j}=\langle i| \rho|j\rangle$ with $i \neq j$. In general, quantum master equations can be written in the form

$$
\begin{equation*}
\partial_{t} \rho_{i j}=\sum_{i^{\prime} j^{\prime}} \mathcal{L}_{i j i^{\prime} j^{\prime}} \rho_{i^{\prime} j^{\prime}}, \tag{2.22}
\end{equation*}
$$

where $\mathcal{L}_{i j i^{\prime} j^{\prime}}$ is a tetradic. Typically, quantum master equations are compactly written using a superoperator $\mathcal{L}$, which is known the Liouvillian or Lindbladian

$$
\begin{equation*}
\partial_{t} \rho=\mathcal{L}[\rho] . \tag{2.23}
\end{equation*}
$$

Consider a closed system with Hamiltonian $H=\sum_{i} \varepsilon_{i}|i \times i|$. From Eq. (2.62), it is clear that $\mathcal{L}[\circ]=-i[H, \circ]$ and that

$$
\begin{equation*}
\mathcal{L}_{i j i^{\prime} j^{\prime}}=-i\left(\varepsilon_{i}-\varepsilon_{j}\right) \delta_{i i^{\prime}} \delta_{j j^{\prime}} \tag{2.24}
\end{equation*}
$$

From Eq. (2.24) we easily see that energy eigenstates are stationary $\partial_{t} \rho_{i i}=0$ and that coherences in the energy eigenbasis gain a phase $\left(\varepsilon_{i}-\varepsilon_{j}\right) t$ over a time $t$. However, not much more can be extracted from the Liouvillian of a closed system. Quantum master equations become really useful when one considers the evolution of open quantum systems that weakly interact with their environment.

Consider that the isolated physical system is composed by two subsystems, say $\mathcal{H}=\mathcal{H}_{\mathrm{S}} \otimes \mathcal{H}_{\mathrm{E}}$, the open quantum system and the environment. In many cases of interest, one wants to evaluate an observable $A_{\mathrm{S}}:=A_{\mathrm{S}} \otimes \mathbf{1}_{\mathrm{E}}$ that only acts on the system Hilbert space $\mathcal{H}_{\mathrm{S}}$. Then, it is enough to compute

$$
\begin{equation*}
\left\langle A_{\mathrm{S}}\right\rangle=\operatorname{tr}\left[\left(A_{\mathrm{S}} \otimes 1_{\mathrm{E}}\right) \rho\right]=\operatorname{tr}_{\mathrm{S}}\left[A_{\mathrm{S}}\left(\operatorname{tr}_{\mathrm{E}} \rho\right)\right]=: \operatorname{tr}_{\mathrm{S}}\left(A_{\mathrm{S}} \rho_{\mathrm{S}}\right) \tag{2.25}
\end{equation*}
$$

where we have defined the reduced state of the system $\rho_{\mathrm{S}}:=\operatorname{tr}_{\mathrm{E}}(\rho)$.
Imagine that we are interested in how the expectation value $\left\langle A_{\mathrm{S}}\right\rangle$ depends on time. Computing the evolution of the state $\rho$ according to Eq. (2.11) can be very inefficient, since the environment is potentially very large. Is it possible to find how the reduced state of the system evolves in time $\partial_{t} \rho_{\mathrm{S}}=\mathcal{L}_{\mathrm{S}}\left[\rho_{\mathrm{S}}\right]$ ? Or, equivalently, can we find an evolution map $\mathcal{E}(t)$ such that $\rho_{\mathrm{S}}(t)=\mathcal{E}(t)\left[\rho_{\mathrm{S}}(0)\right]$ ?

Consider that, initially, the open system and the environment are uncorrelated; that is, $\rho(0)=\rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{E}}(0)$. At time $t=0$, they are put into contact and start evolving together according to Eq. (2.11). Let $\left|r_{i}\right\rangle_{E}$ be the eigenstate of $\rho_{\mathrm{E}}(0)$ with eigenvalue $r_{i}$. Then, at time $t$, the state of the system is

$$
\begin{align*}
\rho_{\mathrm{S}}(t) & =\operatorname{tr}_{\mathrm{E}}\left[\exp (-i H t) \rho_{\mathrm{S}} \otimes \rho_{\mathrm{E}}(0) \exp (i H t)\right] \\
& =\sum_{i j} r_{j}\left\langle r_{i}\right| \exp (-i H t)\left|r_{j}\right\rangle_{\mathrm{E}} \rho_{\mathrm{S}}(0)\left\langle r_{j}\right| \exp (i H t)\left|r_{i}\right\rangle_{\mathrm{E}}^{\dagger} \tag{2.26}
\end{align*}
$$

We now introduce the operators $K_{i j}(t):=\sqrt{r_{j}}\left\langle r_{i}\right| \exp (-i H t)\left|r_{j}\right\rangle_{\mathrm{E}} \in \operatorname{Op}\left(\mathcal{H}_{\mathrm{S}}\right)$, which are known as the Kraus operators, and act on the system Hilbert space. We note that the Kraus operators fulfill the completeness relation $\sum_{i j} K_{i j}(t)^{\dagger} K_{i j}(t)=1_{\mathrm{S}}$ for all times $t$. At $t=0$ one has simply that $\mathcal{E}(t=0)=\mathcal{I}_{\mathrm{S}}$, where $\mathcal{I}_{\mathrm{S}}$ is the identity map on the system space. It is easily checked that, if $H=H_{\mathrm{S}}+H_{\mathrm{E}}$; i.e., the system and the environment do not interact, one recovers the closed system unitary evolution. With that definition, we arrive at the desired result

$$
\begin{equation*}
\rho_{\mathrm{S}}(t)=\mathcal{E}(t)\left[\rho_{\mathrm{S}}(0)\right]=\sum_{i j} K_{i j}(t) \rho_{\mathrm{S}}(0) K_{i j}(t)^{\dagger} \tag{2.27}
\end{equation*}
$$

which is also known as the Kraus decomposition [Kra71]. A theorem by Choi [Cho75] says that any map with a Kraus decomposition is CPTP and, conversely, any CPTP map can be decomposed, although not uniquely, in Kraus operators.

In order to convert Eq. (2.27) into the form of a master equation (2.23), we need to perform two steps. First, we take the derivative of Eq. (2.27) which leads to the relation

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=\partial_{t} \mathcal{E}(t)\left[\rho_{\mathrm{S}}(0)\right] . \tag{2.28}
\end{equation*}
$$

Second, we need the relation between $\rho_{\mathrm{S}}(0)$ in terms of $\rho_{\mathrm{S}}(t)$. This is obtained with the inverse of the evolution map $\mathcal{E}(t)^{-1}$, which we assume it exists, although it is potentially very complicated. This leads to a time-dependent Lindbladian $\mathcal{L}_{\mathrm{S}}(t)$ which leads to the rather formal master equation

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=\mathcal{L}_{\mathrm{S}}(t)\left[\rho_{\mathrm{S}}\right]=\left[\partial_{t} \mathcal{E}(t)\right] \mathcal{E}(t)^{-1}\left[\rho_{\mathrm{S}}\right] . \tag{2.29}
\end{equation*}
$$

Equation (2.29), albeit exact and completely general, is rarely of practical use. In the case of Imposing that $\mathcal{L}_{\mathrm{S}}(t)$ to be time-independent, requires also that

$$
\begin{equation*}
\partial_{t} \mathcal{E}(t)=\mathcal{L}_{\mathrm{S}} \mathcal{E}(t) \tag{2.30}
\end{equation*}
$$

which leads to the simple form $\mathcal{E}(t)=\exp \left(\mathcal{L}_{S} t\right)$. In this case, the dynamics forms a dynamical semigroup; that is, $\mathcal{E}(t) \mathcal{E}\left(t^{\prime}\right)=\mathcal{E}\left(t+t^{\prime}\right)$, and $\mathcal{L}_{\mathrm{S}}$ is guaranteed to have the Gorini-Kossakowski-Sudarshan-Lindblad form [GKS76; Lin76]

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=-i\left[H_{\mathrm{S}}^{\prime}, \rho_{\mathrm{S}}\right]+\sum_{k} \kappa_{k}\left(J_{k} \rho_{\mathrm{S}} J_{k}-\frac{1}{2}\left\{J_{k}^{\dagger} J_{k}, \rho_{\mathrm{S}}\right\}\right), \tag{2.31}
\end{equation*}
$$

with $H_{\mathrm{S}}^{\prime}$ being a Hermitian operator and $\kappa_{k} \geq 0$ being positive. Hence, the potential of quantum master equations for open quantum systems relies on the physically motivated limits on which Eq. (2.29) takes this relatively simple form.

In general, the dynamics of the evolution map $\mathcal{E}(t)$ are very different from the ones of the unitary evolution $\rho_{\mathrm{S}}(t)=\exp \left(-i H_{\mathrm{S}} t\right) \rho_{\mathrm{S}}(0) \exp \left(i H_{\mathrm{S}} t\right)$ that the system would follow when it is decoupled from the environment. For instance, under the non-unitary dynamics $\mathcal{E}(t)$ the system energy $\left\langle H_{S}\right\rangle$ is no-longer a conserved quantity of the evolution. Also, the purity of the state $\operatorname{tr}\left[\rho(t)^{2}\right]$, which was preserved under unitary dynamics, can now evolve with time. This shows that, for open quantum systems, globally preserved properties (like energy or purity) are not locally preserved. From a physical point of view, open quantum systems interact with their environment by exchanging energy and building up system-environment correlations.

To conclude, classical and quantum master equations are not fully disconnected. In certain cases of practical importance, the diagonal elements $\rho_{i i}$ are dynamically decoupled from the coherences $\rho_{i j}$ with $i \neq j$. Then, the quantum master equation (2.22) reduces to the "classical" master equation (2.21) after identifying $w(i \mid j)=\mathcal{L}_{i i j j}$ for $i \neq j$ constrained to $\mathcal{L}_{i i i i}=-\sum_{j \neq i} w(j \mid i)$.

In the next subsections, we study the derivations of several quantum master equations that arise in different physical contexts. Despite the motivation and the assumptions made to derive each of those master equations is in principle different, they always lead to the same formal structure. This motivates the use of a common framework that is able to put those, in principle different, derivations in the same footage. This framework is known as the Nakajima-Zwanzig theory, which is the object of study of the next Section 2.3.

### 2.2.1 The Pauli master equation

The first master equation derived using the rules of quantum mechanics was obtained by Pauli in Ref. [Pau28]. This master equation was derived in order to understand how the energy populations of a many-body system relax to an equilibrium distribution, starting out from some arbitrary initial distribution. Because the Pauli master equation is concerned only with energy populations, albeit describing a quantum evolution process, it has the form of a classical master equation (2.21). The context in which the Pauli master equation is derived is the following. Consider a many-body system whose Hamiltonian is

$$
\begin{equation*}
H=H_{0}+\lambda V \tag{2.32}
\end{equation*}
$$

where $H_{0}$ is some unperturbed Hamiltonian and $\lambda V$ represents a weak pertubation. We denote by $|j\rangle$ unpertubed energy eigenbasis, so that $H_{0}|i\rangle=\varepsilon_{i}|i\rangle$. We are interested in finding an evolution equation for the probabilities $p\left(\varepsilon_{i}\right)=\rho_{i i}$, which become constant in time as $\lambda \rightarrow 0$. For simplicity, we take $V$ to be fully offdiagonal, that is $V_{i i}=0$ for all $i$. Initially, we assume a diagonal density matrix $\rho_{i j}(0)=p\left(\varepsilon_{i} ; 0\right) \delta_{i j}$.

The evolution of the density matrix in the unperturbed energy eigenbasis is

$$
\begin{equation*}
\rho_{i j}(t)=\sum_{l}\langle i| \exp (-i H t)|l\rangle p\left(\varepsilon_{l} ; 0\right)\langle l| \exp (-i H t)|j\rangle \tag{2.33}
\end{equation*}
$$

Pauli hypothesized that, for sufficiently large systems and general interactions $V$, there exists a timescale $\tau_{\text {rpa }}$ such that the complex numbers $\langle i| \exp (-i H t)|l\rangle$ acquire an effectively random phase. Then, averaging over the initial distribution $p\left(\varepsilon_{l} ; 0\right)$
gives rise to approximately diagonal states for all times $t>\tau_{\mathrm{rpa}}$, leading to a closed equation for the probabilities $p\left(\varepsilon_{i}\right)$. This approximation is known as the random phase approximation.

For an initially diagonal state, the exact time dependence of $p\left(\varepsilon_{i} ; t\right)$ after an elapsed time $t$ is given by

$$
\begin{equation*}
\left.p\left(\varepsilon_{i} ; t\right)=\sum_{j} p\left(\varepsilon_{i} ; t \mid \varepsilon_{j}\right) p\left(\varepsilon_{j} ; 0\right):=\sum_{j}\left|\langle i| e^{-i H t}\right| j\right\rangle\left.\right|^{2} p\left(\varepsilon_{j} ; 0\right) . \tag{2.34}
\end{equation*}
$$

We are interested in computing the transition probabilities $p\left(\varepsilon_{i} ; t \mid \varepsilon_{j}\right)$ in the weakperturbation limit. To that end, we use the identity (2.20) for $X=-i H$ and $Y=-i H_{0}$. The resulting identity can be used to find an expansion of $\exp (-i H t)$ in powers of $\lambda$. The first order yields

$$
\begin{equation*}
e^{-i H t}=e^{-i H_{0} t}-i \lambda \int_{0}^{t} d t^{\prime} e^{-i H_{0}\left(t-t^{\prime}\right)} V e^{-i H_{0} t^{\prime}}+\mathcal{O}\left(\lambda^{2}\right) . \tag{2.35}
\end{equation*}
$$

Thus, in the weak-perturbation limit, transition rates between different states $i \neq j$ are given by

$$
\begin{equation*}
\langle i| e^{-i H t}|j\rangle=-\lambda\langle i| V|j\rangle e^{-i \varepsilon_{i} t} \frac{e^{i \omega_{i j} t}-1}{\omega_{i j}}+\mathcal{O}\left(\lambda^{2}\right), \tag{2.36}
\end{equation*}
$$

where we have introduced the transition frequencies $\omega_{i j}=\varepsilon_{i}-\varepsilon_{j}$. Therefore, in the weak-perturbtion limit we obtain

$$
\begin{equation*}
\left.p\left(\varepsilon_{i} ; t \mid \varepsilon_{j}\right)=2 \pi \lambda^{2}|\langle i| V| j\right\rangle\left.\right|^{2} \Delta\left(\omega_{i j}, t\right)+\mathcal{O}\left(\lambda^{3}\right), \tag{2.37}
\end{equation*}
$$

where the function

$$
\begin{equation*}
\Delta(\omega, t)=\frac{2}{\pi} \frac{\sin ^{2}(\omega t / 2)}{\omega^{2}}, \tag{2.38}
\end{equation*}
$$

has been introduced. As a function of $\omega$, the function $\Delta(\omega, t)$ displays a series of peaks of rapidly decaying height. The first peak is at the origin and has height $t^{2} /(2 \pi)$ and width $2 \pi / t$, in such a way that its area scales linearly with $t$. In fact, for any time $t$, the area under the function $\Delta(\omega, t)$ is always exactly $t$. This behavior already shows that the above derivation is not valid for any time $t$, since the transition probability must remain bounded $p\left(\varepsilon_{i} ; t \mid \varepsilon_{j}\right) \leq 1$. In particular, we restrict ourselves to the van Hove limit [Van57], which corresponds $\lambda \rightarrow 0$ and $t \rightarrow \infty$ while $\lambda^{2} t$ remains constant (and small), which leads to meaningful transition probabilities $p\left(\varepsilon_{i} ; t \mid \varepsilon_{j}\right)$ in the weak-coupling limit.

From Eq. (2.37), it is possible to obtain the so-called Fermi golden rule transition probabilities in the limit of large times. Namely,

$$
\begin{equation*}
\lim _{t \rightarrow \infty} \Delta(\omega, t)=\delta(\omega) t \tag{2.39}
\end{equation*}
$$

which has to be dealt with care.
First, the distribution $\delta(\omega)$ only makes sense if the spectrum of the many-body system can be approximated by a continuous distribution. That is, the limit of the infinite system has to be taken before the van Hove limit. Also, equation (2.39) predicts that only transitions that preserve the bare energy $\varepsilon_{i}=\varepsilon_{j}$ are possible in the large time limit. Physically speaking, only transitions that conserve the perturbed energy should be possible, since the Hamiltonian $H=H_{0}+\lambda V$ is a conserved quantity of the exact evolution. From perturbation theory, we obtain that the corrections to the bare energies $\varepsilon_{i}$ are of order $\lambda^{2}$ for $V_{i i}=0$. Hence, we expect that the only transitions that contribute are those whose corresponding transition frequency is of order $\omega_{i j} \sim \mathcal{O}\left(\lambda^{2}\right)$.

We are now ready to write down the Pauli master equation. Let $\tau_{\text {rel }}$ be the timescale of relaxation of the system, and consider elapsed times $\delta t$ such that $\tau_{\text {rel }} \gg \delta t \geq \tau_{\text {rpa }}$. Then, $\delta t$ is small enough to be considered an "infinitesimal" time step, but large enough for the random phase approximation to hold. Hence, from Eq. (2.34)

$$
\begin{align*}
\partial_{t} p\left(\varepsilon_{i}\right) & =\frac{p\left(\varepsilon_{i} ; t+\delta t\right)-p\left(\varepsilon_{i} ; t\right)}{\delta t} \\
& =\sum_{j \neq i}\left(\frac{p\left(\varepsilon_{i} ; \delta t \mid \varepsilon_{j}\right)}{\delta t} p\left(\varepsilon_{j} ; t\right)-\frac{p\left(\varepsilon_{j} ; \delta t \mid i\right)}{\delta t} p\left(\varepsilon_{i} ; t\right)\right) \tag{2.40}
\end{align*}
$$

where we have used that the evolution is unitary to rewrite $p\left(\varepsilon_{i} ; \delta t \mid \varepsilon_{i}\right)=1-$ $\sum_{j \neq i} p\left(\varepsilon_{i} ; \delta t \mid \varepsilon_{j}\right)$. To conclude the derivation, it is only left to define the transition rates

$$
\begin{equation*}
\left.w\left(\varepsilon_{i} \mid \varepsilon_{j}\right)=\frac{p\left(\varepsilon_{i} ; \delta t \mid \varepsilon_{j}\right)}{\delta t}=2 \pi \lambda^{2}|\langle i| V| j\right\rangle\left.\right|^{2} \delta\left(\omega_{i j}\right), \tag{2.41}
\end{equation*}
$$

with the symmetry property $w\left(\varepsilon_{i} \mid \varepsilon_{j}\right)=w\left(\varepsilon_{j} \mid \varepsilon_{i}\right)$, which can be regarded as a consequence of the microscopic reversibility. Thus, we arrive at the Pauli master equation

$$
\begin{equation*}
\partial_{t} p\left(\varepsilon_{i}\right)=\sum_{j \neq i} w\left(\varepsilon_{i} \mid \varepsilon_{j}\right)\left[p\left(\varepsilon_{j} ; t\right)-p\left(\varepsilon_{i} ; t\right)\right] \tag{2.42}
\end{equation*}
$$

The Pauli master equation has found applications in many areas of physics. For instance, it has been used to study the relaxation dynamics of polyatomic molecules [GRF72] or the electron transport in nanostructures [Fis98]. However, the derivation is not fully transparent. It involves several approximations, like the random phase approximation or the van Hove limit, whose range of validity is not clear. We will revisit this derivation below in the context of the Nakajima-Zwanzig theory.

### 2.2.2 The Redfield master equation

The second type of master equation that we discuss is the Redfield master equation [Red57]. This second type of master equation is derived for an open system, and it is genuinely quantum; that is, is a master equation for the full density matrix including its coherences $\left(\rho_{\mathrm{S}}\right)_{i j}$. Redfield derived this master equation to describe the evolution of "a relatively simple system that interacts with a more complicated system that acts as a temperature bath". The bath is regarded as a macroscopic object that is well-described with a collection of few macroscopic parameters such as its temperature or number of particles that are not affected by the system dynamics. To remind ourselves that the environment is a heat bath, we replace the label ' E ' that made reference to the environment, for the label ' B ' that makes reference to the bath. In this sense, he was interested in the irreversible dynamics of a microscopic system (for instance a nuclear spin) that arose from the interaction with a macroscopic environment (for instance the surrounding solid).

The previous theory to describe these systems was derived by Wangsness and Bloch [WB53], where only the diagonal elements in the energy eigenbasis where treated. However, it was known that quantum coherence played an important role in spin systems and Redfield wanted to include those quantum coherences in the theory.

The Redfield equation is derived in the system-environment paradigm. Consider an isolated physical system composed by two subsystems $\mathcal{H}=\mathcal{H}_{\mathrm{S}} \otimes \mathcal{H}_{\mathrm{B}}$ which, once more, we call the open quantum system and the bath. The Hamiltonian of the isolated system can be always divided into $H=H_{\mathrm{S}}+H_{\mathrm{B}}+H_{\text {int }}$ where $H_{\mathrm{S}}=\sum_{i} \varepsilon_{i}\left|i \chi_{i}\right|$ and $H_{\mathrm{B}}=\sum_{k} e_{k}\left|e_{k} X e_{k}\right|$ contain only degrees of freedom of the system and the bath, respectively. The interaction Hamiltonian can be generally written as $H_{\text {int }}=$ $\lambda \sum_{\alpha} S_{\alpha} \otimes B_{\alpha}$, where $S_{\alpha}$ and $B_{\alpha}$ are system and bath operators, respectively. Initially, we consider that the isolated system was found in the state $\rho(0)=\rho_{\mathrm{S}}(0) \otimes \Phi_{\mathrm{B}}(\mathbf{a})$, where $\rho_{\mathrm{S}}(0)$ is an arbitrary initial state of the system, and $\Phi_{\mathrm{B}}(\mathbf{a})$ is an equilibrium state of the bath; that is, $\left[H_{\mathrm{B}}, \Phi_{\mathrm{B}}(\mathbf{a})\right]=0$. The parameters $\mathbf{a}=\left(a_{1}, a_{2}, \cdots\right)$ are a
collection of macroscopic equilibrium parameters that characterize the equilibrium state; for instance, the average energy, the temperature, or the particle number.

Once the equilibrium state of the bath $\Phi_{\mathrm{B}}(\mathbf{a})$ is fixed, it is useful to introduce the 'mean-field' interaction Hamiltonian

$$
\begin{equation*}
H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a}):=\lambda \sum_{\alpha}\left\langle B_{\alpha}\right\rangle_{\mathrm{a}} S_{\alpha}, \tag{2.43}
\end{equation*}
$$

where $\langle\circ\rangle_{\mathrm{a}}=\operatorname{tr}\left[{ }^{\circ} \Phi_{\mathrm{B}}(\mathbf{a})\right]$, is the quantum expectation value with respect to the equilibrium state $\Phi_{\mathrm{B}}(\mathbf{a})$. Consequently, we also define the remaining interaction Hamiltonian as

$$
\begin{equation*}
\lambda V(\mathbf{a}):=H_{\mathrm{int}}-H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a})=\sum_{\alpha} S_{\alpha} \otimes\left(B_{\alpha}-\left\langle B_{\alpha}\right\rangle_{\mathbf{a}}\right) \tag{2.44}
\end{equation*}
$$

and also we define $\delta B_{\alpha}(\mathbf{a}):=B_{\alpha}-\left\langle B_{\alpha}\right\rangle_{\mathbf{a}}$.
We are interested in deriving a quantum master equation for the reduced density matrix $\rho_{\mathrm{S}}=\operatorname{tr}_{\mathrm{B}} \rho$, and we proceed as follows. First, we go to the interaction picture with respect to $H_{\mathrm{a}}=H_{\mathrm{S}}+H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a})+H_{\mathrm{B}}$. Integrating the Liouville-von Neumann equation in that picture yields

$$
\begin{equation*}
\partial_{t} \tilde{\rho}_{\mathbf{a}}(t)=-i \lambda \int_{0}^{t} d t^{\prime}\left[\tilde{V}_{\mathbf{a}}\left(\mathbf{a} ; t^{\prime}\right), \tilde{\rho}_{\mathbf{a}}\left(t^{\prime}\right)\right] \tag{2.45}
\end{equation*}
$$

where the interaction picture depends explicitly on the equilibrium parameters $\mathbf{a}$; for instance, $\tilde{\rho}_{\mathbf{a}}(t)=\exp \left(i H_{\mathbf{a}} t\right) \rho(t) \exp \left(-i H_{\mathbf{a}} t\right)$. Then, we self-consistently replace the $\tilde{\rho}_{\mathbf{a}}\left(t^{\prime}\right)$ within the integral by the expression of $\tilde{\rho}_{\mathbf{a}}(t)$ evaluated at the time $t^{\prime}$. Taking the time-derivative, we arrive at

$$
\begin{equation*}
\partial_{t} \tilde{\rho}_{\mathbf{a}}(t)=-i \lambda\left[\tilde{V}_{\mathbf{a}}(\mathbf{a} ; t), \tilde{\rho}_{\mathbf{a}}(0)\right]-\lambda^{2} \int_{0}^{t} d t^{\prime}\left[\tilde{V}_{\mathbf{a}}(\mathbf{a} ; t),\left[\tilde{V}_{\mathbf{a}}\left(\mathbf{a} ; t^{\prime}\right), \tilde{\rho}_{\mathbf{a}}\left(t^{\prime}\right)\right]\right] . \tag{2.46}
\end{equation*}
$$

Importantly, equation (2.46) is still exact.
We now take advantage of the weak-coupling; that is, we assume that $\lambda$ is a small energy scale. Then, it makes sense to expand Eq. (2.46) in powers of $\lambda$. First, we note that

$$
\begin{equation*}
\rho_{\mathbf{a}}\left(t^{\prime}\right)=e^{i H_{\mathbf{a}} t}\left[e^{i H_{\mathbf{a}}\left(t^{\prime}-t\right)} e^{-i H\left(t^{\prime}-t\right)}\right] \rho(t)\left[e^{i H\left(t^{\prime}-t\right)} e^{-i H_{\mathbf{a}}\left(t^{\prime}-t\right)}\right] e^{-i H_{\mathbf{a}} t}=\rho_{\mathbf{a}}(t)+\mathcal{O}(\lambda) . \tag{2.47}
\end{equation*}
$$

which is true in virtue of the identity (2.20). Of course, for a finite $\lambda$, the fact that the difference $\left|\rho_{\mathbf{a}}(t)-\rho_{\mathbf{a}}\left(t^{\prime}\right)\right| \sim \mathcal{O}(\lambda)$ does not imply that one can disregard it. If we denote by $\tau_{\mathrm{B}}$ the largest time contributing to the integral in Eq. (2.46), then the
condition to ignore the difference is that the product $\lambda \tau_{\mathrm{B}} \ll 1$. We shall return to the discussion about $\tau_{\mathrm{B}}$ below. Now, we return to the Schrödinger picture and take the trace over the bath to arrive at

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}= & -i\left[H_{\mathrm{S}}+H_{\mathrm{S}}^{\operatorname{mf}}(\mathbf{a}), \rho_{\mathrm{S}}\right]-i \lambda \operatorname{tr}_{\mathrm{B}}\left[V(\mathbf{a}), \tilde{\rho}_{\mathbf{a}}(-t)\right] \\
& -\lambda^{2} \int_{0}^{t} d t^{\prime} \operatorname{tr}_{\mathrm{B}}\left[V(\mathbf{a}),\left[\tilde{V}\left(\mathbf{a} ; t^{\prime}-t\right), \rho\right]\right]+\mathcal{O}\left(\lambda^{3}\right) . \tag{2.48}
\end{align*}
$$

where we have used that $\operatorname{tr}_{\mathrm{B}}\left(\left[H_{\mathrm{B}},{ }^{\circ}\right]\right)=0$ and noted that $\tilde{V}_{\mathrm{a}}(\mathbf{a} ; t)=\tilde{V}(\mathbf{a} ; t)+\mathcal{O}(\lambda)$ with the interaction picture with respect to the bare Hamiltonian $H_{0}=H_{\mathrm{S}}+H_{\mathrm{B}}$; that is, $\tilde{V}(\mathbf{a}, t)=\exp \left(i H_{0} t\right) V(\mathbf{a}) \exp \left(-i H_{0} t\right)$. Equation (2.48) is exact to second order in $\lambda$.

We now perform the so-called Born approximation. It stands that, at any time $t$, the actual state of the system-bath composite can be approximated by $\rho(t) \approx \rho_{\mathrm{S}}(t) \otimes \Phi_{\mathrm{B}}(\mathbf{a})$. The Born approximation is well justified for environments that are so large that the dynamics of the open system cannot induce any appreciable change in its state. Then, its initial state $\Phi_{\mathrm{B}}(\mathbf{a})$ remains constant at all times. With this approximation, we obtain

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=-i\left[H_{\mathrm{S}}+H_{\mathrm{S}}^{\operatorname{mf}}(\mathbf{a}), \rho_{\mathrm{S}}\right]-\lambda^{2} \int_{0}^{t} d \tau \operatorname{tr}_{\mathrm{B}}\left[V(\mathbf{a}),\left[\tilde{V}(\mathbf{a} ;-\tau), \rho_{\mathrm{S}} \otimes \Phi_{\mathrm{B}}(\mathbf{a})\right]\right], \tag{2.49}
\end{equation*}
$$

where we have changed variables to $\tau=t-t^{\prime}$. Equation (2.49) is important, and we give it the name of the time-local equation.

The time-local equation is very similar to the Redfield equation, which requires the extra step of sending the upper limit of the time integral to infinity. This is known as the Markov approximation, which transforms the time-local equation, to a time-local and time-independent equation. The Markov approximation is justified if the timescale $\tau_{\mathrm{B}}$ in which the bath correlation function $C_{\alpha \alpha^{\prime}}(\mathbf{a} ; \tau):=$ $\left\langle\delta \tilde{B}_{\alpha}(\mathbf{a} ; \tau)^{\dagger} \delta \tilde{B}_{\alpha^{\prime}} \mathbf{( a )}\right\rangle_{\mathbf{a}}$ decays is much shorter than the timescale of the evolution of the system. Then, at sufficiently long times $t$, one can extend the upper limit of the integral to infinity, since for all times $\tau \gtrsim \tau_{\mathrm{B}}$ the integrand vanishes.

However, for any finite system, the correlation function becomes arbitrarily close to its initial value for sufficiently long times. This phenomenon is known as a Poincaré recurrence, and the first time it occurs is the Poincaré recurrence time $\tau_{\mathrm{P}}$. Therefore, one should keep in mind that the master equation with the Markov approximation is only valid up to times $t \lesssim \tau_{\mathrm{P}}$. Luckily, the Poincaré recurrence time $\tau_{\mathrm{P}}$ is very large for many-body systems. Indeed, under certain assumptions [Ven15], it can be shown to grow doubly exponential with the system size. Then, the Markov approximation is well justified for typical baths, which are many-body systems. To
avoid the problem of recurrences, some authors take the infinite bath limit. In this limit, the Poincaré recurrence time tends to infinity $\tau_{\mathrm{B}} \rightarrow \infty$ and then, the Markov approximation is well justified for all times $t$. In App. A.2, we discuss in more detail the recurrences of the bath correlation function in finite baths and the absence of recurrences for infinite baths.

While taking the infinite bath limit is typically harmless for evaluating the bath correlation functions, it gives the wrong impression that the infinite bath cannot be disturbed due to the interaction with the system. This is not the case for finite baths, which we discuss in detail in the upcoming chapters, and one should be careful before taking the infinite bath limit.

Assuming that the Markov approximation is well justified, we can then proceed sending the upper limit of the time integral to infinity, which brings us to the Redfield equation

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=-i\left[H_{\mathrm{S}}+H_{\mathrm{S}}^{\operatorname{mf}}(\mathbf{a}), \rho_{\mathrm{S}}\right]-\lambda^{2} \int_{0}^{\infty} d \tau \operatorname{tr}_{\mathrm{B}}\left[V(\mathbf{a}),\left[\tilde{V}(\mathbf{a} ;-\tau), \rho_{\mathrm{S}} \otimes \Phi_{\mathrm{B}}(\mathbf{a})\right]\right] . \tag{2.50}
\end{equation*}
$$

The Redfield equation (2.50) can also be written explicitly in terms of the bath correlation functions $C_{\alpha, \alpha^{\prime}}(\mathbf{a} ; \tau)$. To this end, we introduce the eigendecomposition of the system operators $S_{\alpha}$. Namely, we define

$$
\begin{equation*}
S_{\alpha, \omega}:=\sum_{i j}\langle i| S_{\alpha}|j\rangle|i \nmid j| \delta_{\omega, \varepsilon_{j}-\varepsilon_{i}}, \tag{2.51}
\end{equation*}
$$

in such a way that $\tilde{S}_{\alpha}(t)=\sum_{\omega} S_{\alpha, \omega} \exp (-i \omega t)$. Then, using that $V(\mathbf{a})=\sum_{\alpha} S_{\alpha} \otimes \delta B_{\alpha}(\mathbf{a})$ one obtains

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}= & -i\left[H_{\mathrm{S}}+H_{\mathrm{S}}^{\operatorname{mf}}(\mathbf{a}), \rho_{\mathrm{S}}\right] \\
& +\lambda^{2} \sum_{\alpha \alpha^{\prime}} \sum_{\omega} \int_{0}^{\infty} d \tau C_{\alpha \alpha^{\prime}}(\mathbf{a} ; \tau) e^{i \omega \tau}\left(S_{\alpha^{\prime}, \omega} \rho_{\mathrm{S}} S_{\alpha}^{\dagger}-S_{\alpha}^{\dagger} S_{\alpha^{\prime}, \omega} \rho_{\mathrm{S}}\right)+\text { h.c., } \tag{2.52}
\end{align*}
$$

where we have used that $\Phi_{B}(\mathbf{a})$ is an equilibrium state to take advantage of the relation $\left\langle\delta \tilde{B}_{\alpha}(t)^{\dagger} \delta \tilde{B}_{\alpha^{\prime}}\left(t^{\prime}\right)\right\rangle_{\mathbf{a}}=\left\langle\delta \tilde{B}_{\alpha}\left(t-t^{\prime}\right)^{\dagger} \delta B_{\alpha^{\prime}}\right\rangle_{\mathbf{a}}$. This motivates the definition of the operator $\theta_{\alpha}(\mathbf{a}):=\lambda^{2} \sum_{\omega, \alpha^{\prime}} \int_{0}^{\infty} d \tau C_{\alpha \alpha^{\prime}}(\mathbf{a} ; \tau) e^{i \omega \tau} S_{\alpha^{\prime}, \omega}$. Then, the Redfield equation can be compactly cast as

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=-i\left[H_{\mathrm{S}}+H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a}), \rho_{\mathrm{S}}\right]+\sum_{\alpha}\left[\theta_{\alpha}(\mathbf{a}) \rho_{\mathrm{S}} S_{\alpha}^{\dagger}-S_{\alpha}^{\dagger} \theta_{\alpha}(\mathbf{a}) \rho_{\mathrm{S}}+\text { h.c. }\right] . \tag{2.53}
\end{equation*}
$$

Today, the Redfield master equation has been used in nuclear magnetic resonance for more than half a century under the name of Wangsness-Bloch-Redfield
theory (see for instance [Sli13]). However, using the results of Davies [Dav74], it was noticed by Dümcke and Spohn [DS79] that the quantum evolution generated by the Redfield equation is not always completely positive; that is, $\rho_{\mathrm{S}}(t)$ can develop negative eigenvalues. The negativity results from the failure of the Markovian approximation, specially at short times. Commonly there are two solutions are available for this problem. The first, is to use the slippage super-operator [SSO92; GN99], which corrects for the short-time effects restoring the positivity of the Redfield equation. The second is to introduce a third approximation, on top of the Born and Markov approximations, which is known as the secular approximation. This second solution is the subject of the next subsection.

### 2.2.3 The Born-Markov-secular master equation

The third equation that we discuss is known as the Davies [Dav74] or Born-Markovsecular (BMS) master equation. It requires an extra layer of approximation, the secular approximation, which consists in averaging out the fast oscillating terms in the interaction picture, restoring the positivity that the Redfield equation lacked. However, this averaging procedure neglects many dynamical processes, those with zero time average, whose relative importance depends on the physical system under scrutiny. Some physical systems, like quantum optical ones, are well described after the secular approximation. Other systems, like nuclear spins, are not suited by the secular approximation, and are better described by Redfield equation. Hence, it is important to understand the similarities and differences between the two approaches.

We derive the BMS master equation as follows. Frist, from Eq. (2.53), we move back to the interaction picture with respect to $H_{0}=H_{\mathrm{S}}+H_{\mathrm{B}}$

$$
\begin{align*}
\partial_{t} \tilde{\rho}_{\mathrm{S}}(t)= & -i \sum_{\alpha, \omega}\left\langle B_{\alpha}\right\rangle_{\mathrm{a}} e^{-i \omega t}\left[S_{\alpha, \omega}, \tilde{\rho}_{\mathrm{S}}(t)\right]  \tag{2.54}\\
& \sum_{\alpha \alpha^{\prime}} \sum_{\omega, \omega^{\prime}} \Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega) e^{i\left(\omega^{\prime}-\omega\right) t}\left[S_{\alpha^{\prime}, \omega} \tilde{\rho}_{\mathrm{S}}(t) S_{\alpha, \omega^{\prime}}^{\dagger}-S_{\alpha, \omega^{\prime}}^{\dagger} S_{\alpha^{\prime}, \omega} \tilde{\rho}_{\mathrm{S}}(t)\right]+\text { h.c. }
\end{align*}
$$

where $\Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega):=\lambda^{2} \int_{0}^{\infty} d \tau C_{\alpha \alpha^{\prime}}(\mathbf{a} ; \tau) \exp (i \omega \tau)$ is proportional to the half Fourier transform of the bath correlation function. The secular approximation selects the zero frequency components of the above equation which yields

$$
\begin{align*}
\partial_{t} \tilde{\rho}_{\mathrm{S}}(t)= & -i \sum_{\alpha}\left\langle B_{\alpha}\right\rangle_{\mathrm{a}}\left[S_{\alpha, 0}, \tilde{\rho}_{\mathrm{S}}(t)\right]  \tag{2.55}\\
& +\sum_{\alpha \alpha^{\prime}} \sum_{\omega} \Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)\left[S_{\alpha^{\prime}, \omega} \tilde{\rho}_{\mathrm{S}}(t) S_{\alpha, \omega}^{\dagger}-S_{\alpha, \omega}^{\dagger} S_{\alpha^{\prime}, \omega} \tilde{\rho}_{\mathrm{S}}(t)\right]+\text { h.c. }
\end{align*}
$$

The secular approximation is justified as long as the inverse of the minimum energy transition difference of the system $\min \left|\omega-\omega^{\prime}\right|^{-1}$ for $\omega \neq \omega^{\prime}$, whose inverse defines the timescale of the system $\tau_{\mathrm{S}}$, is much smaller than the typical timescale of the bath $\tau_{\mathrm{B}}$; that is $\left|\omega-\omega^{\prime}\right|^{-1} \sim \tau_{\mathrm{S}} \ll \tau_{\mathrm{B}}$. Intuitively, this timescale difference justifies replacing the exponential factor $\exp \left[i\left(\omega-\omega^{\prime}\right) t\right]$ in Eq. (2.54) by its time average $\delta_{\omega, \omega^{\prime}}$. For instance, this timescale separation is found in quantum optical platforms, where typical bath correlation times $\tau_{\mathrm{B}} \sim 10^{-9}$ seconds while inverse optical frequencies $\tau_{\mathrm{s}} \sim 10^{-15}$ seconds[BP02].

Equation (2.55) is already the BMS master equation, however, it is convenient to present it in a different form. To this end, we now introduce the Hermitian and anti-Hermitian parts of the matrix $\Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$ which we define as

$$
\begin{align*}
& \gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)=\Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)+\Gamma_{\alpha^{\prime} \alpha}(\mathbf{a} ; \omega)^{*},  \tag{2.56}\\
& A_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)=\left[\Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)-\Gamma_{\alpha^{\prime} \alpha}(\mathbf{a} ; \omega)^{*}\right] /(2 i) . \tag{2.57}
\end{align*}
$$

Because the bath correlation function has the symmetry $C_{\alpha \alpha^{\prime}}(\mathbf{a} ; \tau)=C_{\alpha^{\prime} \alpha}(\mathbf{a} ;-\tau)$, the corresponding function $\gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$ can be computed alternatively as the Fourier transform $\gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)=\lambda^{2} \int_{\mathbb{R}} C_{\alpha \alpha^{\prime}}(\mathbf{a} ; \tau) \exp (i \omega \tau)$.

Moving back to the Schrödinger picture, we arrive at the equation

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}= & -i\left[H_{\mathrm{S}}+H_{\mathrm{S}, 0}^{\mathrm{mf}}(\mathbf{a})+H_{\mathrm{S}}^{\mathrm{LS}}(\mathbf{a}), \rho_{\mathrm{S}}\right] \\
& +\lambda^{2} \sum_{\alpha \alpha^{\prime}} \sum_{\omega} \gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)\left(S_{\alpha^{\prime}, \omega} \rho_{\mathrm{S}} S_{\alpha, \omega}^{\dagger}-\frac{1}{2}\left\{S_{\alpha, \omega}^{\dagger} S_{\alpha^{\prime}, \omega}, \rho_{\mathrm{S}}\right\}\right), \tag{2.58}
\end{align*}
$$

where the Hamiltonian terms

$$
\begin{align*}
& H_{\mathrm{S}, 0}^{\mathrm{mf}}(\mathbf{a})=\lambda \sum_{\alpha}\left\langle B_{\alpha}\right\rangle_{\mathbf{a}} S_{\alpha, 0},  \tag{2.59}\\
& H_{\mathrm{S}}^{\mathrm{LS}}(\mathbf{a})=\lambda^{2} \sum_{\alpha \alpha^{\prime}} \sum_{\omega} A_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega) S_{\alpha, \omega}^{\dagger} S_{\alpha^{\prime}, \omega}, \tag{2.60}
\end{align*}
$$

that commute with the bare system Hamiltonian $H_{S}$, have been defined. For historical reasons, we have labeled with the subscript 'LS' the third term, which stands for the Lamb-shift Hamiltonian. Hereafter, for compactness of the notation, we gather all the Hamiltonians into $H_{\mathrm{S}}^{\prime}(\mathbf{a})=H_{\mathrm{S}}+H_{\mathrm{S}, 0}^{\mathrm{mf}}(\mathbf{a})+H_{\mathrm{S}}^{\mathrm{LS}}(\mathbf{a})$.

Finally, we recall that the rates $\gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$ are Hermitian, and therefore, can be diagonalized. Let $u_{\alpha \beta}(\mathbf{a} ; \omega)$ be the components of the unitary matrix that diagonalizes $\gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$; that is, $\gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)=u_{\beta \alpha^{\prime}}^{*}(\mathbf{a} ; \omega) u_{\beta \alpha^{\prime}}(\mathbf{a} ; \omega) \kappa_{\beta}(\mathbf{a} ; \omega)$. Defining the jump
operators $J_{\beta, \omega}(\mathbf{a}):=\sum_{\alpha} u_{\beta \alpha}(\mathbf{a}) S_{\alpha, \omega}$, we arrive at the final BMS master equation

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}= & -i\left[H_{\mathrm{S}}^{\prime}(\mathbf{a}), \rho_{\mathrm{S}}\right]+\sum_{\beta, \omega} \kappa_{\beta}(\mathbf{a} ; \omega)\left(J_{\beta, \omega}(\mathbf{a}) \rho_{\mathrm{S}} J_{\beta, \omega}(\mathbf{a})^{\dagger}-\frac{1}{2}\left\{J_{\beta, \omega}(\mathbf{a})^{\dagger} J_{\beta, \omega}(\mathbf{a}), \rho_{\mathrm{S}}\right\}\right) \\
& =: \mathcal{L}_{\mathrm{S}}\left[\rho_{\mathrm{S}}\right] . \tag{2.61}
\end{align*}
$$

The Lindbladian $\mathcal{L}_{\mathrm{S}}$ is time-independent, which implies that the evolution map $\mathcal{E}(t)$ under the BMS master equation has the simple form $\mathcal{E}(t)=\exp \left(\mathcal{L}_{S} t\right)$. In this simplified form, it is easy to see that Eq. (2.61) becomes compatible with Eq. (2.29). Finally, it can be shown using Bochner's theorem [BP02; RH12] that $\kappa_{\beta}(\mathbf{a} ; \omega) \geq 0$, which guarantees that Eq. (2.61) has the form of the well-known Gorini-Kossakowski-Sudarshan-Lindblad [GKS76; Lin76], which ensures that $\rho_{\mathrm{S}}$ is positive at all times.

### 2.3 The Nakajima-Zwanzig theory

The aim of this section is to introduce the theory derived by Nakajima and Zwanzig in Refs. [Nak58; Zwa60; Zwa61]. The Nakajima-Zwanzig theory is based on identifying the relevant part of the dynamics; which is problem dependent, in a mathematically well-defined manner, and then, exploit the linearity of the Liouville-von Neumann equation to obtain an equation of motion that involves only the relevant part. The greatest advantage of this formulation is that it unifies the derivation of numerous master equations. As an illustration of the potential of the NakajimaZwanzig techniques, we derive the master equations discussed throughout the last section as particular applications of the theory.

We start introducing $\mathcal{P}$, a time-independent linear map on the Hilbert space $\mathcal{H}$ as well as its complementary map $\mathcal{Q}:=\mathcal{I}-\mathcal{P}$. Hereafter, the maps $\mathcal{P}$ and $\mathcal{Q}$ are referred to as the relevant and irrelevant map, respectively. For instance, if the relevant part of the dynamics is the reduced state of the system $\rho_{\mathrm{S}}$, the relevant map $\mathcal{P}$ corresponds basically to a partial trace over the environment of the total state $\rho$. We consider an isolated system whose microscopic description is encoded in the time-dependent Hamiltonian $H(t)$. Even if the Hamiltonian $H$ is time-independent, the time-dependent formulation of the Nakajima-Zwanzig equation can be useful to derive master equations in the interaction picture. Then, the system evolves accordingly to the Liouville-von Neumann equation

$$
\begin{equation*}
\partial_{t} \rho=-i[H(t), \rho]=: \mathcal{L}(t)[\rho] . \tag{2.62}
\end{equation*}
$$

Since the relevant $\mathcal{P}$ and irrelevant $\mathcal{Q}$ map add up to the identity, it is possible to decompose the Liouville-von Neumann equation as

$$
\begin{align*}
& \partial_{t} \mathcal{P} \rho=\mathcal{P} \mathcal{L}(t) \mathcal{P} \rho+\mathcal{P} \mathcal{L}(t) \mathcal{Q} \rho,  \tag{2.63}\\
& \partial_{t} \mathcal{Q} \rho=\mathcal{Q} \mathcal{L}(t) \mathcal{P} \rho+\mathcal{Q} \mathcal{L}(t) \mathcal{Q} \rho, \tag{2.64}
\end{align*}
$$

where, hereafter, we omit the square brackets to lighten the notation. Equation (2.63) is a differential equation for the relevant part $\mathcal{P} \rho$, but it still depends on the irrelevant part of the state $\mathcal{Q} \rho$. We can eliminate the dependence on $\mathcal{Q} \rho$ as follows. First, we formally integrate Eq. (2.64) and obtain

$$
\begin{equation*}
\mathcal{Q} \rho(t)=\mathcal{G}(t, 0) \mathcal{Q} \rho(0)+\int_{0}^{t} d t^{\prime} \mathcal{C}\left(t, t^{\prime}\right) \mathcal{Q} \mathcal{L}\left(t^{\prime}\right) \mathcal{P} \rho\left(t^{\prime}\right) . \tag{2.65}
\end{equation*}
$$

where we have introduced the propagator (or Green's function)

$$
\begin{equation*}
\mathcal{G}\left(t, t_{0}\right)=\exp _{+}\left[\int_{t_{0}}^{t} \mathcal{Q} \mathcal{L}\left(t^{\prime}\right) d t^{\prime}\right], \tag{2.66}
\end{equation*}
$$

where $\exp _{+}\left({ }^{\circ}\right)$ corresponds to the time-ordered exponential. And second, we substitute Eq. (2.65) into Eq. (2.63) to arrive at the Nakajima-Zwanzig equation

$$
\begin{equation*}
\partial_{t} \mathcal{P} \rho=\mathcal{P} \mathcal{L}(t) \mathcal{P} \rho+I(t)+\int_{0}^{t} d t^{\prime} \mathcal{K}\left(t, t^{\prime}\right) \mathcal{P} \rho\left(t^{\prime}\right) \tag{2.67}
\end{equation*}
$$

where the inhomogeneous term

$$
\begin{equation*}
I(t)=\mathcal{P} \mathcal{L}(t) \mathcal{G}(t, 0) \mathcal{Q} \rho(0) \tag{2.68}
\end{equation*}
$$

and the memory kernel

$$
\begin{equation*}
\mathcal{K}\left(t, t^{\prime}\right)=\mathcal{P} \mathcal{L}(t) \mathcal{G}\left(t, t^{\prime}\right) \mathcal{Q} \mathcal{L}\left(t^{\prime}\right), \tag{2.69}
\end{equation*}
$$

have been defined. In the simpler case of a time-independent Hamiltonian $H(t)=H$, the Liouvillian becomes time-independent $\mathcal{L}(t)=\mathcal{L}$ and the propagator is simply $\mathcal{G}\left(t, t_{0}\right)=\mathcal{G}\left(t-t_{0}\right)=\exp \left[\mathcal{Q L}\left(t-t_{0}\right)\right]$. As a consequence, the kernel $\mathcal{K}\left(t, t^{\prime}\right)=\mathcal{K}\left(t-t^{\prime}\right)$ becomes also a function of the time difference only.

The Nakajima-Zwanzig equation (2.67) is an exact equation for the relevant part of state $\mathcal{P} \rho$. It has several interesting properties. First, given a map $\mathcal{P}$, there is a class of initial states $\rho(0)$ for which the Nakajima-Zwanzig becomes particularly simple. Namely, if the initial state is invariant under the action of the map; that is, $\rho(0)=\mathcal{P} \rho(0)$, the inhomogeneous term $I(t)=0$ vanishes for all times. Then,
the Nakajima-Zwanzig equation becomes a closed equation for the relevant part $\mathcal{P} \rho$. Second, the memory kernel $\mathcal{K}\left(t, t^{\prime}\right)$ can capture the non-Markovian features of the evolution. And third, in certain scenarios, the information leakage out of the relevant subspace gives rise to an effective irreversible dynamics for $\mathcal{P} \rho$.

Despite being exact, the Nakajima-Zwanzig equation cannot always be solved. For a weakly perturbed Hamiltonian $H=H_{0}+\lambda V$, one can find a formal solution to the Nakajima-Zwanzig equation in terms of an infinite series, but very rarely can be resumed to produce a closed expression for $\mathcal{P} \rho(t)$. We discuss in some depth this procedure in App. A.1. Hence, one has to rely on numerical techniques to obtain the relevant dynamics or, crucially, use Eq. (2.67) as a starting point to implement problem-dependent approximation schemes. Such approximations schemes correspond to the identification of the relevant map $\mathcal{P}$ and a perturbation parameter $\lambda$, for which it is justified to truncate the expansion at some finite order.

A good choice of the relevant map $\mathcal{P}$ is one such that the relevant state $\mathcal{P} \rho$ is low dimensional and a good approximation for the actual state $\rho$. The "low dimensional" part ensures that the dynamics can be solved efficiently; that is, with limited computational resources. The "good approximation" part is tightly connected with the desired property of a time-local equation. In other words, for the state $\rho(t+d t)$ is fully determined by the state at the previous time-step $\rho(t)$, and we would like this property to be transferred as much as possible to $\mathcal{P} \rho(t+d t)$ and $\mathcal{P} \rho(t)$. Clearly, $\mathcal{P}$ should be a compromise between the "low dimensional" and the "good approximation" parts. For instance, $\mathcal{P}[\circ]=\operatorname{tr}[\odot] 1 / d$ gives a zerodimensional description, but is a bad approximation; while, $\mathcal{P}[\circ]=\mathcal{I}[\circ]$ is a perfect approximation, but makes the Nakajima-Zwanzig equation identical to the Liouvillevon Neumann equation which is practically impossible to solve.

In the following, to illustrate the applicability of the Nakajima-Zwanzig theory, we study perturbative expansions of the Nakajima-Zwanzig equation for different choices of the relevant map $\mathcal{P}$. Those choices correspond to the Pauli, Redfield, and BMS master equation discussed in Sec. 2.2.

### 2.3.1 Revisiting the Pauli master equation

The first application of Nakajima-Zwanzig theory is to provide a compelling derivation of the Pauli master equation for a diagonal state $\rho(0)$, and the Hamiltonian in Eq. (2.32). We decompose the Liouvillian operator as $\mathcal{L}=\mathcal{L}_{0}+\lambda \mathcal{L}_{1}$, corresponding to the zeroth and first order in $\lambda$ contributions, respectively. To be precise $\mathcal{L}_{0}[\circ]=-i[H, \circ]$ and $\mathcal{L}_{1}[\circ]=-i[V, \circ]$. We are interested in a master equation for the diagonal elements of the density matrix. Hence, we define the relevant projection
operator

$$
\begin{equation*}
\mathcal{D}[\rho]:=\sum_{i}\langle i| \rho|i\rangle|i \times i|, \tag{2.70}
\end{equation*}
$$

which fulfills the property $\mathcal{D}^{2}=\mathcal{D}$. Its components, as well as the ones for the irrelevant map $\mathcal{I}-\mathcal{D}$, are given by

$$
\begin{align*}
& \mathcal{D}_{i i^{\prime} j^{\prime}}=\delta_{i i^{\prime}} \delta_{j j^{\prime}} \delta_{i j},  \tag{2.71}\\
& {[(\mathcal{I}-\mathcal{D})]_{i i^{\prime} j^{\prime}}=\delta_{i i^{\prime}} \delta_{j j^{\prime}}\left(1-\delta_{i j}\right) .} \tag{2.72}
\end{align*}
$$

Hence, when acting onto a quantum map $\mathcal{M}$, the relevant map $\mathcal{D}$ selects the components $(\mathcal{D M})_{i j i^{\prime} j^{\prime}}=\mathcal{M}_{i i i^{\prime} j^{\prime}}$. It is also useful to write the components of the total and unperturbed Liouvillian

$$
\begin{align*}
& \mathcal{L}_{i j i^{\prime} j^{\prime}}=-i\left(\langle i| H\left|i^{\prime}\right\rangle \delta_{j j^{\prime}}-\left\langle j^{\prime}\right| H|j\rangle \delta_{i i^{\prime}}\right),  \tag{2.73}\\
& \left(\mathcal{L}_{0}\right)_{i i^{\prime} j^{\prime}}=-i\left(\varepsilon_{i}-\varepsilon_{j}\right) \delta_{i i^{\prime}} \delta_{j j^{\prime}} . \tag{2.74}
\end{align*}
$$

Using the above properties, we obtain $\mathcal{D} \mathcal{L D}=0$, and noting that $\mathcal{D}[\rho(0)]=\rho(0)$, the Nakajima-Zwanzig equation simplifies into

$$
\begin{equation*}
\partial_{t} \mathcal{D}[\rho]=\int_{0}^{t} d t^{\prime} \mathcal{K}\left(t-t^{\prime}\right) \mathcal{D}\left[\rho\left(t^{\prime}\right)\right], \tag{2.75}
\end{equation*}
$$

or, in terms of the components of the density matrix

$$
\begin{equation*}
\partial_{t} \rho_{i i}=\sum_{j} \int_{0}^{t} d t^{\prime}\left[\mathcal{K}\left(t-t^{\prime}\right)\right]_{i i j j} \rho_{j j}\left(t^{\prime}\right) . \tag{2.76}
\end{equation*}
$$

Equation (2.76) starts looking like a master equation. The master equation structure can be made even more apparent by noting the sum rule $\sum_{i^{\prime}} \mathcal{L}_{i j i^{\prime} i^{\prime}}=0$, which can be used to cast $[\mathcal{K}(t)]_{i i i i}=-\sum_{j \neq i}[\mathcal{K}(t)]_{i i j j}$. Then, identifying $p\left(\varepsilon_{i}\right)=\rho_{i i}$, and introducing the change of variables $\tau=t-t_{1}$, we arrive at

$$
\begin{equation*}
\partial_{t} p\left(\varepsilon_{i}\right)=\sum_{j \neq i} \int_{0}^{t} d \tau[\mathcal{K}(\tau)]_{i j j}\left[p\left(\varepsilon_{j} ; t-\tau\right)-p\left(\varepsilon_{i} ; t-\tau\right)\right] . \tag{2.77}
\end{equation*}
$$

where no approximation has been done.
In the standard derivation of the Pauli master equation (see Sec. 2.2.1), we introduced the timescale $\tau_{\lambda}:=\lambda^{2} t$ in the context of the van Hove limit. To take
this limit, it is helpful to introduce the probability distributions $P\left(\varepsilon_{i} ; \tau_{\lambda}\right)=p\left(\varepsilon_{i} ; t\right)$. This transforms Eq. (2.77) to

$$
\begin{equation*}
\partial_{\tau_{\lambda}} P\left(\varepsilon_{i}\right)=\sum_{j \neq i} \int_{0}^{\tau_{\lambda} / \lambda^{2}} d \tau \lambda^{-2}[\mathcal{K}(\tau)]_{i j j}\left[P\left(\varepsilon_{j} ; \tau_{\lambda}-\lambda^{2} \tau\right)-P\left(\varepsilon_{i} ; \tau_{\lambda}-\lambda^{2} \tau\right)\right], \tag{2.78}
\end{equation*}
$$

which is still exact. Now, Eq. (2.78) is ready for taking the van Hove limit: $\lambda \rightarrow 0$, $t \rightarrow \infty$, and $\tau_{\lambda}=\lambda^{2} t=$ constant, which brings it to the master equation form

$$
\begin{equation*}
\partial_{\tau_{\lambda}} P\left(\varepsilon_{i}\right)=\sum_{j \neq i} \int_{0}^{\infty} d \tau \lambda^{-2}[\mathcal{K}(\tau)]_{i i j j}\left[P\left(\varepsilon_{j} ; \tau_{\lambda}\right)-P\left(\varepsilon_{i} ; \tau_{\lambda}\right)\right] . \tag{2.79}
\end{equation*}
$$

After taking the limit, we can transform back to the original probabilities $p\left(\varepsilon_{i} ; t\right)$ which leads to

$$
\begin{align*}
\partial_{t} p\left(\varepsilon_{i}\right) & =\sum_{j \neq i} \int_{0}^{\infty} d \tau[\mathcal{K}(\tau)]_{i j j}\left[p\left(\varepsilon_{j} ; t\right)-p\left(\varepsilon_{i} ; t\right)\right] \\
& =\sum_{j \neq i} w\left(\varepsilon_{i} \mid \mathcal{g}_{j}\right)\left[p\left(\varepsilon_{j} ; t\right)-p\left(\varepsilon_{i} ; t\right)\right] \tag{2.80}
\end{align*}
$$

where we have identified the transition rates $w\left(\varepsilon_{i} \mid \varepsilon_{j}\right)$ as the integrated components of the memory kernel.

It is only left to compute explicitly the transition rates $w\left(\varepsilon_{i} \mid \varepsilon_{j}\right)$ for $j \neq i$. First, we note the properties $\left(\mathcal{L}_{0}\right)_{i i i i^{\prime} j^{\prime}}=0$, and $\left[(\mathcal{I}-\mathcal{D}) \mathcal{L}_{0}\right]_{i j i^{\prime} i^{\prime}}=0$, which are a consequence of $\mathcal{D} \mathcal{L}_{0}=0$. Then, the memory kernel simplifies into

$$
\begin{equation*}
\mathcal{K}(t)=\lambda^{2} \mathcal{L}_{1} \exp \left[(\mathcal{I}-\mathcal{D})\left(\mathcal{L}_{0}+\lambda \mathcal{L}_{1}\right) t\right](\mathcal{I}-\mathcal{D}) \mathcal{L}_{1} . \tag{2.81}
\end{equation*}
$$

Now, we take advantage of the weak-perturbation limit, which allows to expand

$$
\begin{equation*}
\mathcal{K}(t)=\lambda^{2} \mathcal{L}_{1} \exp \left(\mathcal{L}_{0} t\right)(\mathcal{I}-\mathcal{D}) \mathcal{L}_{1}+\mathcal{O}\left(\lambda^{3}\right), \tag{2.82}
\end{equation*}
$$

where we have used again that $\mathcal{D} \mathcal{L}_{0}=0$. Note also that the exponential of the unperturbed Liouvillian has the components $\left[\exp \left(\mathcal{L}_{0} t\right)\right]_{i i^{\prime} j^{\prime}}=\exp \left(-i \omega_{i j} t\right) \delta_{i i^{\prime}} \delta_{j j^{\prime}}$. Hence, taking $i \neq j$, we arrive at

$$
\begin{align*}
w\left(\varepsilon_{i} \mid \varepsilon_{j}\right) & =\lambda^{2} \sum_{k l}\left(\mathcal{L}_{1}\right)_{i k l}\left[(\mathcal{I}-\mathcal{D}) \mathcal{L}_{1}\right]_{k l j j} \int_{0}^{\infty} d \tau e^{-i \omega_{k l} \tau} \\
& \left.=2 \pi \lambda^{2}|\langle i| V| j\right\rangle\left.\right|^{2} \delta\left(\omega_{i j}\right), \tag{2.83}
\end{align*}
$$

which corresponds to the "Golden rule" transition rates obtained in Sec. 2.2.1. The present derivation of the Pauli master equation, this time through NakajimaZwanzig theory, is much more transparent since no random phase approximation was done, and the van Hove limit appears in a mathematically well-defined way. The only persistent pathology of the present formulation is that a $\delta$-function appears without having introduced the notion of a continuous spectrum. Namely, for a finite system with a discrete spectrum, the $\delta$-function is meaningless.

### 2.3.2 Revisiting the Redfield equation

The second application of the Nakajima-Zwanzig theory is the to derive the Redfield equation (2.50). The setup is the same as in Sec. 2.2.2. Namely, we divide the Hamiltonian of the isolated system into $H=H_{\mathrm{S}}+H_{\mathrm{B}}+H_{\text {int }}$ where $H_{\mathrm{S}}=\sum_{i} \varepsilon_{i}|i \times i|$ and $H_{\mathrm{B}}=\sum_{k} e_{k}\left|e_{k} X e_{k}\right|$ contain only degrees of freedom of the system and the bath, respectively. We also decompose $H_{\text {int }}=\lambda \sum_{\alpha} S_{\alpha} \otimes B_{\alpha}$, where $S_{\alpha}$ and $B_{\alpha}$ are system and bath operators, respectively. We denote by $H_{0}=H_{\mathrm{S}}+H_{\mathrm{B}}$ the zeroth order in $\lambda$ of the Hamiltonian and decompose $\mathcal{L}=\mathcal{L}_{0}+\lambda \mathcal{L}_{1}$; that is, $\mathcal{L}_{0}\left[{ }^{\circ}\right]=-i\left[H_{0}, \circ\right]$, while $\mathcal{L}_{1}=-i \lambda^{-1}\left[H_{\text {int }}, \circ\right]$. Initially, we consider that the isolated system is in the state $\rho(0)=$ $\rho_{\mathrm{S}}(0) \otimes \Phi_{\mathrm{B}}(\mathbf{a})$, where $\rho_{\mathrm{S}}(0)$ is an arbitrary initial state of the system, and $\Phi_{\mathrm{B}}(\mathbf{a})$ is an equilibrium state of the bath; that is, $\left[H_{\mathrm{B}}, \Phi_{\mathrm{B}}(\mathbf{a})\right]=0$. The parameters $\mathbf{a}=\left(a_{1}, a_{2}, \cdots\right)$ are macroscopic equilibrium parameters that characterize the equilibrium state; for instance, the energy, the temperature, or the particle number. We are interested in the dynamics of the reduced state of the system $\rho_{\mathrm{S}}=\operatorname{tr}_{\mathrm{B}}(\rho)$. Accordingly, we define the relevant projection operator

$$
\begin{equation*}
\mathcal{B}[\rho]:=\operatorname{tr}_{\mathrm{B}}(\rho) \otimes \Phi_{\mathrm{B}}(\mathbf{a}) . \tag{2.84}
\end{equation*}
$$

We are now ready to evaluate all terms appearing in the Nakajima-Zwanzig equation (2.67) term by term. Because we are interested in the evolution equation of $\rho_{\mathrm{S}}$, rather than $\mathcal{B}[\rho]$, we can first trace over the bath to obtain

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=\operatorname{tr}_{\mathrm{B}}(\mathcal{B L} \mathcal{L} \rho)+\operatorname{tr}_{\mathrm{B}}[I(t)]+\int_{0}^{t} d t^{\prime} \operatorname{tr}_{\mathrm{B}}\left[\mathcal{K}\left(t-t^{\prime}\right) \mathcal{B} \rho\left(t^{\prime}\right)\right] . \tag{2.85}
\end{equation*}
$$

We start noting that, for our choice of initial state $\rho(0)$, we find that the inhomogeneous term vanishes $I(t)=0$ for all times $t$. Next, we compute

$$
\begin{equation*}
\mathcal{B L} \mathcal{B} \rho=\left(-i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}\right]-i \lambda\left[\sum_{\alpha}\left\langle B_{\alpha}\right\rangle_{\mathbf{a}} S_{\alpha}, \rho_{\mathrm{S}}\right]\right) \otimes \Phi_{\mathrm{B}}(\mathbf{a}) \tag{2.86}
\end{equation*}
$$

At this point, many authors decide to assume for simplicity that $\left\langle B_{\alpha}\right\rangle_{\mathbf{a}}=0$, which can be done without loss of generality. We intentionally keep track of this term since it will become important in the upcoming chapters. We take the opportunity to define $\delta B_{\alpha}(\mathbf{a})=B_{\alpha}-\left\langle B_{\alpha}\right\rangle_{\mathbf{a}}, H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a}):=\lambda \sum_{\alpha}\left\langle B_{\alpha}\right\rangle_{\mathbf{a}} S_{\alpha}$, where ' mf ' stands for mean-field, and $\lambda \mathrm{V}(\mathbf{a}):=H_{\text {int }}-H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a})$.

For the convolution term, we have to evaluate the memory kernel $\mathcal{K}(t)$, whose expression is relatively involved. Here, we take advantage of the weak-coupling limit and compute the kernel only to second order in $\lambda$. We start computing the terms

$$
\begin{align*}
& (\mathcal{I}-\mathcal{B}) \mathcal{L} \mathcal{B}[\circ]=-i \lambda\left[V(\mathbf{a}), \operatorname{tr}_{\mathrm{B}}(\circ) \otimes \Phi_{\mathrm{B}}(\mathbf{a})\right],  \tag{2.87}\\
& \mathcal{B L}(\mathcal{I}-\mathcal{B})[\circ]=-i \lambda \operatorname{tr}_{\mathrm{B}}([V(\mathbf{a}), \circ]) \otimes \Phi_{\mathrm{B}}(\mathbf{a}), \tag{2.88}
\end{align*}
$$

where we have used the properties $\operatorname{tr}_{\mathrm{B}}\left(\left[H_{\mathrm{B}}, \circ\right]\right)=0, \operatorname{tr}_{\mathrm{B}}\left(\left[H_{\mathrm{S}}, \circ\right]\right)=\left[H_{\mathrm{S}}, \operatorname{tr}_{\mathrm{B}}(\circ)\right]$, and the fact that $\Phi_{\mathrm{B}}(\mathbf{a})$ is an equilibrium state of the bath $\left[H_{\mathrm{B}}, \Phi_{\mathrm{B}}(\mathbf{a})\right]=0$. Therefore, to second order in $\lambda$ we can substitute in the exponential $\mathcal{L}$ by $\mathcal{L}_{0}$. The exponent is explicitly given by

$$
\begin{equation*}
(\mathcal{I}-\mathcal{B}) \mathcal{L}_{0}\left[\left[_{0}\right]=\mathcal{L}_{0}\left[\left[^{\circ}\right]+i\left[H_{S}, \operatorname{tr}_{\mathrm{B}}(\circ) \otimes \Phi_{\mathrm{B}}(\mathbf{a})\right],\right.\right. \tag{2.89}
\end{equation*}
$$

and a quick calculation shows that in fact

$$
\begin{equation*}
\exp \left[(\mathcal{I}-\mathcal{B}) \mathcal{L}_{0} t\right](\mathcal{I}-\mathcal{B}) \mathcal{L}_{1} \mathcal{B} \rho=\exp \left(\mathcal{L}_{0} t\right)(\mathcal{I}-\mathcal{B}) \mathcal{L}_{1} \mathcal{B} \rho \tag{2.90}
\end{equation*}
$$

which follows from $\operatorname{tr}_{\mathrm{B}}\left[\delta B_{\alpha}(\mathbf{a}) \Phi_{\mathrm{B}}(\mathbf{a})\right]=0$, and $\operatorname{tr}_{\mathrm{B}}\left(\left[H_{\mathrm{B}}, \circ\right]\right)=0$. The map $\exp \left(\mathcal{L}_{0} t\right)\left[{ }^{\circ}\right]=$ $\exp \left(-i H_{0} t\right) \circ \exp \left(i H_{0} t\right)$ and, hence, we identify $\tilde{X}(t)=\exp \left(-\mathcal{L}_{0} t\right)[X(0)]$ as the interaction picture with respect to $H_{0}$. Finally, we make use of $\exp \left[-i H_{0}\left(t-t^{\prime}\right)\right] \exp \left(-i H t^{\prime}\right)=$ $\exp (-i H t)+\mathcal{O}(\lambda)$ to arrive at the time-local equation

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=-i\left[H_{\mathrm{S}}+H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a}), \rho_{\mathrm{S}}\right]-\lambda^{2} \int_{0}^{t} d t^{\prime} \operatorname{tr}_{\mathrm{B}}\left\{\left[V(\mathbf{a}),\left[\tilde{V}\left(\mathbf{a} ; t^{\prime}-t\right), \rho_{\mathrm{S}} \otimes \Phi_{\mathrm{B}}(\mathbf{a})\right]\right]\right\} \tag{2.91}
\end{equation*}
$$

which is identical to equation (2.49). Importantly, we have arrived to Eq. (2.91) without making use of any approximation other than a weak-coupling expansion in $\lambda$. From Eq. (2.91), one can proceed analogously to Sec. 2.2.2 and Sec. 2.2.3 to derive the Redfield and BMS master equations.

### 2.3.3 Outlook on Nakajima-Zwanzig theory

The Nakajima-Zwanzig theory is a powerful technique to derive quantum master equations. Its power resides in its versatility. The crucial insight about this theory
is that one can use an arbitrary linear and time-independent map $\mathcal{P}$ to decompose the Liouville-von Neumann equation (2.62) into the two mutually dependent equations (2.63) and (2.64). Then, injecting the formal solution of Eq. (2.64) into Eq. (2.63) one arrives to the Nakajima-Zwanzig equation (2.67) which is a closed equation for the relevant state $\mathcal{P} \rho$.

The task of the physicist is, then, finding a clever choice of $\mathcal{P}$ from which the relevant information about the dynamics can be extracted. However, since the Nakajima-Zwanzig equation is basically a rearranged version of the Liouville-von Neumann equation, solving it is virtually impossible. Hence, the choice of $\mathcal{P}$ has to be also one that, given a physical problem, can help to simplify the NakajimaZwanzig equation to made it tractable. Customary choices of $\mathcal{P}$ correspond to projection maps $\mathcal{P}^{2}=\mathcal{P}$ such that make the initial state $\rho(0)$ invariant under the projection $\mathcal{P} \rho(0)=\rho(0)$. Then, the inhomogeneous term $I(t)$ vanishes for all times $t$. In open quantum systems, the decomposition between system and bath degrees of freedom can be regarded as part of the choice of $\mathcal{P}$. Basically, the bath can be regarded as the part of the isolated system that you trace over. Hence, a good partition is one such that the interaction between the parts is weak, which allows for an expansion in the interaction strength $\lambda$ along the lines of Sec. 2.2.2 and Sec. 2.2.3.

Given the choices $\mathcal{P}=\mathcal{D}$ and $\mathcal{P}=\mathcal{B}$ that we used to derive the Pauli and Redfield master equations, respectively, it may seem that $\mathcal{P}$ can only select certain components of the exact density matrix $\rho$. As it turns out, it can do much more than that. For instance, in many quantum systems the noise can be described by a stochastic process. In the simplest case, the stochastic process enters the description as a stochastic term $\eta(t) V$ in the Hamiltonian; that is, $H=H_{0}+\eta(t) V$ (see for instance [Cai19]). Then, the evolution of the density matrix becomes a function of the noise realization $\rho_{\eta}$. If one is interested on the average trajectory $\rho=\mathbb{E}\left[\rho_{\eta}\right]$, where $\mathbb{E}[\circ]$ represents the average over the noise realizations, one can use the projection $\mathcal{P}[\circ]=\mathbb{E}[\circ]$ to derive the corresponding quantum master equation. The Nakajima-Zwanzig equation can be used even in the classical context. For instance, in its pioneering work [Zwa60], Zwanzig discussed the possibility of using the projector $\mathcal{P}[\circ]=\left[\int d q^{3 N}\right]^{-1} \int d q^{3 N}$, where $q$ here denotes a canonical coordinate of a particle, to obtain the momentum dependence of the phase-space distribution of a classical system of $N$ particles.

### 2.4 Typical bath examples

In this section, we discuss briefly the typical models for the bath Hamiltonian $H_{\mathrm{B}}$ and the interaction Hamiltonian $H_{\text {int }}$. The aim is, for each model, to compute explicitly $\Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$ as well as its 'Hermitian' $\gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$ and 'anti-Hermitian' $A_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$ parts. Because for the typical models below, the interaction has the simpler form $H_{\text {int }}=$ $\lambda S \otimes B$, we drop the indices $\alpha \alpha^{\prime}$ during the computation.

### 2.4.1 A bath of harmonic oscillators

The first example we discuss is a bath of harmonic oscillators, also known as bosonic bath, or the Caldeira-Leggett bath [CL83]. This bath consists of a collection of $N_{b}$ non-interacting harmonic oscillators or bosons $r=1, \cdots, N_{b}$ with corresponding bosonic operators $b_{r}$ and $b_{r}^{\dagger}$ that fulfill the canonical commutation relations $\left[b_{r}, b_{r^{\prime}}\right]=0$, and $\left[b_{r}, b_{r^{\prime}}^{\dagger}\right]=\delta_{r r^{\prime}} 1$. Then, the bath Hamiltonian is

$$
\begin{equation*}
H_{\mathrm{B}}=\sum_{r=1}^{N_{b}} \Omega_{r}\left(b_{r}^{\dagger} b_{r}+\mathbf{1} / 2\right), \tag{2.92}
\end{equation*}
$$

where $\Omega_{r} \geq 0$ is the frequency of the $r^{\text {th }}$ oscillator. The interaction is taken of the form

$$
\begin{equation*}
H_{\mathrm{int}}=\lambda S \otimes B=\lambda S \otimes \sum_{r=1}^{N_{b}} c_{r}\left(b_{r}^{\dagger}+b_{r}\right), \tag{2.93}
\end{equation*}
$$

where $c_{r}$ is the coupling strength to the $r^{\text {th }}$ oscillator and $S$ is an arbitrary system operator. The interaction (2.93) is also known as "position-type" interaction, since the combination $\left(b_{r}^{\dagger}+b_{r}\right)$ is proportional to the position operator of a bosonic system.

For each boson $b_{r}$, we introduce the orthonormal Fock basis $\left|n_{r}\right\rangle$, with $n_{r}=$ $0,1, \cdots$ with $\left\langle m_{r} \mid n_{r}\right\rangle=\delta_{m n}$. The action of the bosonic operators onto the Fock basis elements is $b_{r}\left|n_{r}\right\rangle=n_{r}\left|n_{r}-1\right\rangle$ and $b_{r}^{\dagger}\left|n_{r}\right\rangle=\left(n_{r}+1\right)\left|n_{r}+1\right\rangle$. Then, an energy eigenstate $|\mathbf{n}\rangle=\left|n_{1}, \cdots, n_{r}, \cdots, n_{N_{b}}\right\rangle$ has energy $E_{\mathbf{n}}=\sum_{r} n_{r} \Omega_{r}+E_{0}$, where the zero-point energy $E_{0}:=N_{b} / 2 \sum_{r} \Omega_{r}$ is the energy of the vacuum state $|\mathbf{0}\rangle$. It is not hard to see that the coupling operator is off-diagonal in this energy eigenbasis; that is, $\langle\mathbf{n}| B|\mathbf{n}\rangle=0$. Then, we find $\delta B(\mathbf{a})=B$ for any equilibrium state $\Phi_{\mathrm{B}}(\mathbf{a})$. Also, it is easy to see that $\tilde{b}_{r}(t)=\exp \left(i H_{B} t\right) b_{r} \exp \left(-i H_{B} t\right)=b_{r} \exp \left(-i \Omega_{r} t\right)$. Then, the bath correlation function for this model is simply

$$
\begin{equation*}
C(\mathbf{a} ; \tau)=\sum_{r} c_{r}^{2}\left(\operatorname{tr}_{r}\left\{b_{r}^{\dagger} b_{r} \operatorname{tr}_{r}\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]\right\} e^{i \Omega_{r} \tau}+\operatorname{tr}_{r}\left\{b_{r} b_{r}^{\dagger} \operatorname{tr}_{\gamma}\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]\right\} e^{-i \Omega_{r} \tau}\right), \tag{2.94}
\end{equation*}
$$

where $\operatorname{tr}_{\gamma^{\prime}}(\circ)$ denotes taking the trace over every boson except the $r^{\text {th }}$ one. Interestingly, to compute the $r^{\text {th }}$ spin contribution to the correlation function, only the reduced state of $\Phi_{\mathrm{B}}(\mathbf{a})$ of the $r^{\text {th }}$ subsystem is needed. Note that the collection of reduced states $\left\{\Phi_{r}(\mathbf{a}):=\operatorname{tr}_{\gamma}\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]\right\}$ contains much less information than the full state $\Phi_{\mathrm{B}}(\mathbf{a})$.

To proceed further, one has to specify the equilibrium state $\Phi_{B}(\mathbf{a})$. The most typical choice corresponds to the Gibbs state $\pi_{\mathrm{B}}(\beta):=\exp \left(-\beta H_{\mathrm{B}}\right) / Z_{\mathrm{B}}(\beta)$, where $Z_{\mathrm{B}}(\beta)=\operatorname{tr}\left[\exp \left(-\beta H_{B}\right)\right]$ is the canonical partition function. The Gibbs state $\pi_{\mathrm{B}}(\beta)$ depends on a single parameter $\mathbf{a}=(\beta)$, which is the inverse temperature. Then, we find

$$
\begin{equation*}
C(\beta ; \tau)=\sum_{r} c_{r}^{2}\left\{n_{b}\left(\beta, \Omega_{r}\right) e^{i \Omega_{r} \tau}+\left[n_{b}\left(\beta, \Omega_{r}\right)+1\right] e^{-i \Omega_{r} \tau}\right\} \tag{2.95}
\end{equation*}
$$

where $n_{b}(\beta, \Omega):=[\exp (\beta \Omega)-1]^{-1}$ is the bosonic occupation number.
We are ultimately interested in the functions $\gamma(\mathbf{a} ; \omega)$ and $A(\mathbf{a} ; \omega)$, which, for a single bath operator, correspond to the real and imaginary part of $\Gamma(\mathbf{a} ; \omega)$. Hence, we have to compute

$$
\begin{equation*}
\Gamma(\beta ; \omega)=\lim _{t \rightarrow \infty} \lambda^{2} \int_{0}^{t} d \tau \sum_{r=1}^{N_{b}} c_{r}^{2}\left\{n_{b}\left(\beta, \Omega_{r}\right) e^{i\left(\omega+\Omega_{r}\right) \tau}+\left[n_{b}\left(\beta, \Omega_{r}\right)+1\right] e^{i\left(\omega-\Omega_{r}\right) \tau}\right\} \tag{2.96}
\end{equation*}
$$

Before taking the limit, one can sum first over the oscillators $r$ or integrate over time yielding the same result. However, things become subtle after taking the limit $t \rightarrow \infty$. On the one hand, if one decides to first integrate over time, the integrand does is simply an oscillating phase which does not converge. On the other hand, if one sum first over the oscillators $r$, many phases with different weights enter the sum. Then, the integrand becomes a rapidly decaying function of time, which seem to converge for long but finite times $t$. However, we know that, for any finite number $N_{b}$ (even countably infinite; see App. A.2), the correlation function exhibits quasi periodic revivals known as Poincaré recurrences. Formally, the only solution is taking the infinite bath limit, for which the correlation function shows no revivals.

To proceed with the computation, we first introduce the spectral density $J(\Omega):=$ $2 \pi \lambda^{2} \sum_{r=1}^{N_{b}} c_{r}^{2} \delta\left(\Omega-\Omega_{r}\right)$, which helps to do a smooth transition to the infinite bath limit. The spectral density $J(\Omega)$ can be regarded as an unnormalized distribution of bath oscillators weighted by the corresponding coupling strength squared. Then, we recast Eq. (2.96) as

$$
\begin{equation*}
\Gamma(\beta ; \omega)=\int_{0}^{\infty} \frac{d \Omega}{2 \pi} J(\Omega) \int_{0}^{\infty} d \tau\left\{n_{b}(\beta, \Omega) e^{i(\omega+\Omega) \tau}+\left[n_{b}(\beta, \Omega)+1\right] e^{i(\omega-\Omega) \tau}\right\} \tag{2.97}
\end{equation*}
$$

To compute the integral, we take advantage of the Sokhotski-Plemelj theorem, which, for the case we consider, stands that

$$
\begin{equation*}
\int d x f(x) \lim _{\epsilon \rightarrow 0^{+}} \int_{0}^{\infty} d y e^{i(x+i \epsilon) y}=\pi f(0)+i \mathrm{PV} \int \frac{f(x)}{x} d x \tag{2.98}
\end{equation*}
$$

where PV stands for the Cauchy 'Principal Value'. This relation is relatively easy to prove, since the left-hand side of Eq. (2.98) amounts to

$$
\begin{align*}
\text { LHS } & =\int d x f(x) \lim _{\epsilon \rightarrow 0^{+}} \frac{\epsilon+i x}{x^{2}+\epsilon^{2}} \\
& =\pi \int d x f(x) \lim _{\epsilon \rightarrow 0^{+}}\left[\frac{1}{\pi} \frac{\epsilon}{x^{2}+\epsilon^{2}}\right]+i \int f(x) \lim _{\epsilon \rightarrow 0^{+}} \frac{x}{x^{2}+\epsilon^{2}} . \tag{2.99}
\end{align*}
$$

The object between brackets in the first term is identified as a normalized Lorentzian, which tends to a $\delta(x)$ as $\epsilon$ tends to zero. In the second term, the pole at $x=0$ is removed symmetrically around the origin, which yields the principal value of the integral.

We apply now the Sokhotski-Plemelj theorem to Eq. (2.97) to obtain the closed expression

$$
\begin{align*}
\Gamma(\beta ; \omega)= & \frac{1}{2}\left\{\theta(-\omega) J(-\omega) n_{b}(\beta,-\omega)+\theta(\omega) J(\omega)\left[1+n_{b}(\beta, \omega)\right]\right\} \\
& +i \operatorname{PV} \int_{0}^{\infty} \frac{d \Omega}{2 \pi} J(\Omega)\left[\frac{n_{b}(\beta, \Omega)}{\omega+\Omega}+\frac{1+n_{b}(\beta, \Omega)}{\omega-\Omega}\right], \tag{2.100}
\end{align*}
$$

where $\theta(\omega)$ is the Heaviside step function. Equation (2.100) can be simplified further noting the following properties. First, the bosonic occupation number fulfills $n_{b}(\beta,-\omega)=-1-n_{b}(\beta, \omega)$. Second, the spectral density $J(\Omega)$ is only evaluated for positive frequency arguments, so we can extend it towards negative frequencies as an odd function; that is, $J(-\Omega):=-J(\Omega)$. Combining both properties, we can compactly write

$$
\begin{equation*}
\Gamma(\beta ; \omega)=\frac{J(\omega)}{2}\left[1+n_{b}(\beta, \omega)\right]+i \operatorname{PV} \int_{\mathbb{R}} \frac{d \Omega}{2 \pi} \frac{J(\Omega)\left[1+n_{b}(\beta, \Omega)\right]}{\omega-\Omega} \tag{2.101}
\end{equation*}
$$

Then, identifying the real and imaginary parts with the functions $\gamma(\beta ; \omega)$ and $A(\beta ; \omega)$ we arrive at our final result

$$
\begin{align*}
& \gamma(\beta ; \omega)=J(\omega)\left[1+n_{b}(\beta, \omega)\right]  \tag{2.102}\\
& A(\beta ; \omega)=\operatorname{PV} \int_{\mathbb{R}} \frac{d \Omega}{2 \pi} \frac{J(\Omega)\left[n_{b}(\beta, \Omega)+1\right]}{\omega-\Omega} \tag{2.103}
\end{align*}
$$

To conclude, we remark that, strictly speaking, the expressions in Eqs. (2.102) and Eq. (2.103) are only valid for an infinite bath. Although each boson lives in an infinite dimensional Hilbert space, a single boson does not constitute an infinite bath, instead, to derive Eqs. (2.102) and Eq. (2.103) we needed a continuous spectral density $J(\Omega)$. However, one expects those expressions to hold even for a finite bath provided that the bath correlation time $\tau_{\mathrm{B}}$ is small and only times $t$ smaller than the Poincaré recurrence time $\tau_{\mathrm{P}}$ are considered. In that scenario, $J(\Omega)$ should be replaced by its coarse-grained approximation in the same way one replaces continuous probability distributions by histograms of discrete probability distributions.

### 2.4.2 A bath of spins

The second example of a bath that we discuss corresponds to a bath of independent spins. This is model is referred to as the independent spin bath, or simply the spin bath, although much more sophisticated versions of the model considered here go under the same name (see [PS00]). The spin bath consists of a collection of $N_{s}$ non-interacting spins $r=1, \cdots, N_{s}$ with corresponding spin (Pauli) operators $\sigma_{r}^{x, y, z}$ that fulfill the spin commutation relations $\left[\sigma_{r}^{\mu}, \sigma_{r^{\prime}}^{\nu}\right]=2 i \delta_{r r^{\prime}} \sum_{\xi=x, y, z} \epsilon^{\mu v \xi} \sigma_{r}^{\xi}$, where $\epsilon^{\mu \nu \xi}$ is the Levi-Civita tensor. The bath Hamiltonian is simply

$$
\begin{equation*}
H_{\mathrm{B}}=\sum_{r=1}^{N_{s}} \frac{\Omega_{r}}{2} \sigma_{r}^{z} \tag{2.104}
\end{equation*}
$$

where $\Omega_{r}$ is the spin transition frequency (or Zeeman frequency) of the $r^{\text {th }}$ spin, and the interaction is taken to be

$$
\begin{equation*}
H_{\mathrm{int}}=\lambda S \otimes B=\lambda S \otimes \sum_{r=1}^{N_{s}} c_{r} \sigma_{r}^{x} \tag{2.105}
\end{equation*}
$$

where $c_{r}$ is the coupling strength to the $r^{\text {th }}$ spin.
For each spin, we introduce the energy eigenbasis $\left|n_{r}\right\rangle$ where $n_{r}= \pm 1$, and fulfills $\sigma_{r}^{z}\left|n_{r}\right\rangle=n_{r}\left|n_{r}\right\rangle$. Energy eigenstates are then given by $|\mathbf{n}\rangle=\left|n_{1}, \cdots, n_{r}, \cdots, n_{N_{s}}\right\rangle$ and have energy $E_{\mathbf{n}}=\sum_{r} n_{r} \Omega_{r} / 2$. It is not hard to see that, again, we have $\delta B(\mathbf{a})=B$ for any equilibrium state $\Phi_{\mathrm{B}}(\mathbf{a})$. For this model, the correlation function yields

$$
\begin{equation*}
C(\mathbf{a} ; \tau)=\sum_{r=1}^{N_{s}}\left\{\operatorname{tr}_{r}\left[\sigma_{r}^{+} \sigma_{r}^{-} \Phi_{r}(\mathbf{a})\right] e^{i \Omega_{r} t}+\operatorname{tr}_{r}\left\{\sigma_{r}^{-} \sigma_{r}^{+} \Phi_{r}(\mathbf{a})\right] e^{-i \Omega_{r} t}\right\} . \tag{2.106}
\end{equation*}
$$

where $\sigma_{r}^{+}=\left|+_{r} X-_{r}\right|=\sigma_{r}^{-\dagger}$ and, again, $\Phi_{r}(\mathbf{a}):=\operatorname{tr}_{\gamma}\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]$.

Once more, we consider the equilibrium state $\Phi_{\mathrm{B}}(\mathbf{a})$ to be a Gibbs state $\pi_{\mathrm{B}}(\beta):=$ $\exp \left(-\beta H_{\mathrm{B}}\right) / Z_{\mathrm{B}}(\beta)$ at inverse temperature $\beta$. Introducing the Fermionic occupation number $n_{f}(\beta, \Omega)=[\exp (\beta \Omega)+1]^{-1}$, we arrive at

$$
\begin{equation*}
C(\beta ; \tau)=\sum_{r} c_{r}^{2}\left\{n_{f}\left(\beta, \Omega_{r}\right) e^{i \Omega_{r} \tau}+\left[1-n_{f}\left(\beta, \Omega_{r}\right)\right] e^{-i \Omega_{r} \tau}\right\} \tag{2.107}
\end{equation*}
$$

which is very similar to Eq. (2.95). We can now proceed with the same discussion of the previous Section 2.4.1. We use the spectral density $J(\Omega)=2 \pi \lambda^{2} \sum_{r} c_{r}^{2} \delta\left(\Omega-\Omega_{r}\right)$ to make a smooth transition to the infinite bath, and use the Sokhotski-Plemelj theorem (2.98) to derive a closed expression for $\Gamma(\beta ; \omega)$. There is the caveat that the Fermionic occupation number fulfills $n_{f}(\beta, \omega)=1-n_{f}(\beta, \omega)$ and, therefore, one has to extend the spectral density as an even function towards negative frequencies; that is, $J(-\Omega):=J(\Omega)$. Then, one arrives at

$$
\begin{equation*}
\Gamma(\beta ; \omega)=\frac{\lambda^{2}}{2} J(\omega)\left[1-n_{f}(\beta, \omega)\right]+i \mathrm{PV} \int_{\mathbb{R}} \frac{d \Omega}{2 \pi} \frac{J(\Omega)\left[1-n_{f}(\beta, \Omega)\right]}{\omega-\Omega} \tag{2.108}
\end{equation*}
$$

from which we identify

$$
\begin{align*}
& \gamma(\beta ; \omega)=J(\omega)\left[1-n_{f}(\beta, \omega)\right]  \tag{2.109}\\
& A(\beta ; \omega)=\operatorname{PV} \int_{\mathbb{R}} \frac{d \Omega}{2 \pi} \frac{J(\Omega)\left[1-n_{f}(\beta, \Omega)\right]}{\omega-\Omega} \tag{2.110}
\end{align*}
$$

To conclude, we remark once more that, strictly speaking, Eqs. (2.109) and (2.110) are only valid in the infinite bath limit, but we expect those expressions to coincide with the finite bath value for times $t$ smaller than the Poincare recurrence time $\tau_{\mathrm{P}}$.

### 2.5 General properties of master equations

In this section, we briefly discuss some general properties of quantum master equations, which help to understand which is the typical dynamics of open quantum systems.

### 2.5.1 Contractivity and the stationary state

Consider two quantum states $\rho$ and $\sigma$, a quantum evolution $\mathcal{E}(t)$. We use the convention that $\rho(t):=\mathcal{E}(t)[\rho(0)]$. We ask the following question. Are $\rho$ and $\sigma$ "closer" or "further apart" after evolving a time $t$ under the evolution $\mathcal{E}(t)$ ? Naively, it seems that the answer should depend on $\rho, \sigma$, and/or the map $\mathcal{E}(t)$. It turns out
that states always come closer together after a general evolution $\mathcal{E}(t)$. We say that CPTP maps are contractive.

However, for the above statement to make sense, we need to define first a notion of distance between quantum states. We start by introducing the "trace norm". Let $X=X^{\dagger}$ be a Hermitian operator in $\operatorname{Op}(\mathcal{H})$ with (possibly degenerated) real eigenvalues $x$ and an eigenbasis $\{|x\rangle\}$. We define the trace norm of X as

$$
\begin{equation*}
\operatorname{tr}|X|:=\operatorname{tr} \sqrt{X^{\dagger} X}=\sum_{x}|x| \geq 0 . \tag{2.111}
\end{equation*}
$$

As a side remark, we note that the trace norm is also defined for non-Hermitean operators, since the combination $X^{\dagger} X \geq 0$ can be always diagonalized. Given the trace norm, we define the "trace distance" between two states $\rho$ and $\sigma$ as

$$
\begin{equation*}
d_{\mathrm{tr}}(\rho, \sigma):=\operatorname{tr}|\rho-\sigma| . \tag{2.112}
\end{equation*}
$$

So far, we have only defined evolution maps $\mathcal{E}(t)$ for positive time arguments $t \geq 0$, which are CPTP. We now are in the position to prove that CPTP maps are contractive. First, we decompose the Hermitian operator $X=X_{+}-X_{-}$where $X_{+}=\sum_{x \geq 0} x|x X x|$ and $X_{-}=\sum_{x<0} X_{-}$, where both are positive operators. Second, we note the chain of inequalities

$$
\begin{align*}
\operatorname{tr}|\mathcal{E}(t)[X]| & =\operatorname{tr}\left|\mathcal{E}(t)\left[X_{+}\right]-\mathcal{E}(t)\left[X_{-}\right]\right| \\
& \leq \operatorname{tr}\left|\mathcal{E}(t)\left[X_{+}\right]\right|+\operatorname{tr}\left|\mathcal{E}(t)\left[X_{-}\right]\right| \\
& =\operatorname{tr}\left|X_{+}\right|+\operatorname{tr}\left|X_{-}\right|=\operatorname{tr}|X|, \tag{2.113}
\end{align*}
$$

that is, for any time $t \geq 0$ the trace norm of $X$ is smaller or equal than its original value. Finally, let $X=\rho-\sigma$ and let to conclude that $d_{\mathrm{tr}}(\rho(0), \sigma(0)) \geq d_{\mathrm{tr}}(\rho(t), \sigma(t))$, which concludes the proof. It is important to keep in mind that the inverse map $\mathcal{E}(-t)=\mathcal{E}^{-1}(t)$, which propagates backwards in time, is not completely-positive.

Now we restrict ourselves to quantum evolution maps of the form $\mathcal{E}(t)=$ $\exp (\mathcal{L} t)$, which are known are dynamical semigroups. The crucial property of dynamical semigroups is that, given two times $t_{1}$ and $t_{2}$, the evolution map fulfills $\mathcal{E}\left(t_{1}+t_{2}\right)=\mathcal{E}\left(t_{1}\right) \mathcal{E}\left(t_{2}\right)$. Now, take $t_{1}=t \geq 0$ and $t_{2}=t+\delta t$, with $\delta t>0$. Then, we have $d_{\mathrm{tr}}(\rho(t), \sigma(t)) \geq d_{\mathrm{tr}}(\rho(t+\delta t), \sigma(t+\delta t))$. Hence, the contractivity property is stronger for dynamical semigroups; that is, two arbitrary states come closer together at every time step $\delta t>0$.

Very much related to the notion of contractivity there is the notion of stationary state. Given $\mathcal{E}(t)=\exp (\mathcal{L} t)$, we say that $\rho^{\text {st }}$ is stationary if $\mathcal{E}(t)\left[\rho^{\text {st }}\right]=\rho^{\text {st }}$ or, equivalently, if $\mathcal{L}\left(\rho^{\text {st }}\right)=0$. For stationary states, the contractivity property implies that $d_{\mathrm{tr}}\left(\rho^{\mathrm{st}}, \sigma(0)\right) \geq d_{\mathrm{tr}}\left(\rho^{\mathrm{st}}, \sigma(t)\right)$.

It turns out that the trace-preserving condition guarantees that every $\mathcal{L}$ has, at least, one stationary state. The proof only requires basic algebra and the vectorization procedure of Sec. 2.1.5. First, using the vectorization procedure, we map $\mathcal{L}[\rho] \mapsto \mathcal{L}|\rho\rangle\rangle$. In general, $\mathcal{L}$ corresponds to a non-Hermitian matrix. Nonetheless, it has a characteristic polynomial $\operatorname{det}\left(\mathcal{L}-\lambda_{\mu} \mathcal{I}\right)=0$, whose roots correspond to the eigenvalues $\lambda_{\mu}$. The corresponding generalized eigenvectors have the so-called 'left' or 'right' character, which corresponds to

$$
\begin{align*}
& \left.\left.\mathcal{L}\left|R_{\mu}\right\rangle\right\rangle=\lambda_{\mu}\left|R_{\mu}\right\rangle\right\rangle,  \tag{2.114}\\
& \left\langle\left\langle L_{\mu}\right| \mathcal{L}=\left\langle\left\langle L_{\mu}\right| \lambda_{\mu},\right.\right. \tag{2.115}
\end{align*}
$$

which can be chosen with the bi-orthonormal property $\left\langle\left\langle L_{\mu} \mid R_{\nu}\right\rangle\right\rangle=\delta_{\mu v}$. Now, we note that because $\mathcal{L}$ is trace preserving, it follows that $\operatorname{tr}(\mathcal{L}[X])=0$ for all $X$. But then, $\langle<\mathbf{1}|$ must be a left generalized eigenvector of eigenvalue $\left\langle<L_{1}\right|$ with eigenvalue $\lambda_{1}=0$; that is, $\langle\langle\mathbf{1}| \mathcal{L}=0$, since $\langle\langle\mathbf{1}| \mathcal{L} \mid X\rangle\rangle=0$ vanishes for all $X$. Then, the corresponding right eigenvector $R_{1}=\rho^{\text {st }}$ is a stationary state because it fulfills $\mathcal{L}\left[R_{1}\right]=0$. We shall revisit the spectral properties of the Lindbladian in Chap. 5.

To conclude, CPTP maps are contractive, which means that an application of the map reduces the distance between arbitrary pairs of states. If the evolution map forms a dynamical semigroup, like for the BMS master equation, then the distance between a pair of states is reduced at every time step. Then, for sufficiently long times $t$ arbitrary quantum states converge towards the stationary state (or multiple stationary quantities).

### 2.5.2 Population dynamics and coherence decay

In general, the evolution of open quantum systems couples the evolution of the populations $p\left(\varepsilon_{i}\right)=\left(\rho_{\mathrm{S}}\right)_{i i}$ and the coherences $\left(\rho_{\mathrm{S}}\right)_{i j}$ with $i \neq j$. This means that the evolution of one influences the other. When the dynamics of the populations and the coherences decouple, the populations follow a classical master equation of the form (2.21). An example of decoupled dynamics is the Pauli master equation, which gives no information about the dynamics of the coherences. Here, we discuss how the evolution of the populations $p\left(\varepsilon_{i}\right)$ and the coherences $\left(\rho_{\mathrm{S}}\right)_{i j}$ in the bare system eigenbasis $\{|i\rangle\}$ influence each other in the case of the Redfield and the BMS master equation. Within this section, to keep the notation light, we denote $\left(\rho_{\mathrm{S}}\right)_{i j}$ simply as $\rho_{i j}$.

We start with the Redfield equation (2.53). It is convenient to use tetradic notation to write down the Redfield equation in terms of the Redfield tetradic (or Redfield tensor) $R_{i j k l}(\mathbf{a})$ in such a way that the $i j^{\text {th }}$ element of the Redfield equation
is

$$
\begin{equation*}
\partial_{t} \rho_{i j}=-i\left(\varepsilon_{i}-\varepsilon_{j}\right) \rho_{i j}+\sum_{k l} R_{i j k l}(\mathbf{a}) \rho_{k l} \tag{2.116}
\end{equation*}
$$

where the Redfield tetradic yields

$$
\begin{align*}
R_{i j k l}(\mathbf{a}):= & -i\left[H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a})_{i k} \delta_{l j}-H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a})_{l j} \delta_{i k}\right]  \tag{2.117}\\
& +\sum_{\alpha \alpha^{\prime}}\left[\Gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{k i}\right) S_{\alpha^{\prime}, i k}\left(S_{\alpha, j l}\right)^{*}-\delta_{j l} \sum_{m} \Gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{k m}\right)\left(S_{\alpha, m i}\right)^{*} S_{\alpha^{\prime}, m k}+\text { c.c. }\right]
\end{align*}
$$

One can interpret the Redfield tetradic $R_{i j k l}(\mathbf{a})$ as the correction to the unitary dynamics due to the presence of the environment, which weakly couples to the system. For instance, the influence of the populations onto themselves is given by the components

$$
\begin{equation*}
R_{i i j j}(\mathbf{a})=\sum_{\alpha \alpha^{\prime}}\left[\gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{j i}\right) S_{\alpha^{\prime}, i j}\left(S_{\alpha, i j}\right)^{*}-\delta_{i j} \sum_{k} \gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{i k}\right)\left(S_{\alpha, k i}\right)^{*} S_{\alpha^{\prime}, k i}\right], \tag{2.118}
\end{equation*}
$$

where we have used (2.56). However, from Eq. (2.117), the elements $R_{i k l}(\mathbf{a})$ that describe the influence of the coherences $\rho_{k l}$ on the populations are, in general, not zero. Hence, we conclude that for the Redfield equation, the dynamics of the populations depend on the coherences.

We consider now the BMS master equation, which corresponds to performing the secular approximation to the Redfield equation. To avoid getting lost into details, we shall focus now on non-degenerate systems with non-degenerate transitions for which $\varepsilon_{i}=\varepsilon_{j}$ implies $i=j$ and $\omega_{i k}=\omega_{j l}$ implies $i=j$ and $k=l$. This is often justified since exact degeneracies are relatively rare. Nonetheless, we refer the interested reader to Ref. [BES16] for an enlarged discussion including the possibility of degenerate eigenstates and transitions. Following Sec. 2.2.3, this procedure leads to Eq. (2.58). Denoting by $R_{i j k l}^{\text {sec }}(\mathbf{a})$ the Redfield tensor after the secular approximation, we find

$$
\begin{align*}
R_{i j l l}^{\mathrm{sec}}(\mathbf{a}):= & -i\left\{\left[H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a})+H_{\mathrm{S}}^{\mathrm{LS}}(\mathbf{a})\right]_{i i}-\left[H_{\mathrm{S}}^{\mathrm{mf}}(\mathbf{a})-H_{\mathrm{S}}^{\mathrm{LS}}(\mathbf{a})\right]_{j j}\right\} \delta_{i k} \delta_{j l}  \tag{2.119}\\
& +\sum_{\alpha \alpha^{\prime}}\left\{\gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{k i}\right) S_{\alpha^{\prime}, i k}\left(S_{\alpha, j l}\right)^{*} \delta_{i j} \delta_{k l}\right. \\
& \left.-\left(\delta_{i k} \delta_{j l} / 2\right) \sum_{m n}\left(\delta_{n i}+\delta_{n j}\right) \gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{n m}\right)\left(S_{\alpha, m n}\right)^{*} S_{\alpha^{\prime}, m n}\right\} .
\end{align*}
$$

From the Redfield tensor after the secular approximation, we can obtain the equation of motion for the populations $\partial_{t} p\left(\varepsilon_{i}\right)=\sum_{k l}{ }_{i i k l}^{\sec }(\mathbf{a}) \rho_{k l}$. Then, the elements that contribute to the dynamics are of the tetradic yield

$$
\begin{equation*}
R_{i i k l}^{\mathrm{sec}}(\mathbf{a})=\delta_{k l} \sum_{\alpha \alpha^{\prime}}\left[\gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{k i}\right) S_{\alpha^{\prime}, i k}\left(S_{\alpha, j l}\right)^{*}-\delta_{i k} \sum_{m} \gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{i m}\right)\left(S_{\alpha, m i}\right)^{*} S_{\alpha^{\prime}, m i}\right] . \tag{2.120}
\end{equation*}
$$

Because $R_{i i k l}^{\text {sec }}(\mathbf{a})=0$ for $k \neq l$, the populations evolve autonomously according to the classical master equation Eq. (2.21) with the transition rates

$$
\begin{equation*}
w\left(\mathbf{a} ; \varepsilon_{i} \mid \varepsilon_{j}\right)=\sum_{\alpha \alpha^{\prime}} \gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{j i}\right) S_{\alpha^{\prime}, i j}\left(S_{\alpha, i j}\right)^{*} . \tag{2.121}
\end{equation*}
$$

Similarly, one finds that the coherences evolve autonomously, since $R_{i j k k}^{\text {sec }}(\mathbf{a})=0$ for all $i \neq j$. Hence, under the BMS master equation, both the populations and the coherences evolve independently of each other. A quick calculation reveals that, for $i \neq j$, one has

$$
\begin{equation*}
\partial_{t} \rho_{i j}=\left\{-i \omega_{i j}^{\prime}(\mathbf{a})-\sum_{\alpha \alpha^{\prime}} \sum_{k l}\left(\delta_{i l}+\delta_{j l}\right) \gamma_{\alpha \alpha^{\prime}}\left(\mathbf{a} ; \omega_{l m}\right)\left(S_{\alpha, m l}\right)^{*} S_{\alpha^{\prime}, m l}\right\} \rho_{i j}, \tag{2.122}
\end{equation*}
$$

where $\omega_{i j}^{\prime}(\mathbf{a})=H_{\mathrm{s}}^{\prime}(\mathbf{a})_{i i}-H_{\mathrm{S}}^{\prime}(\mathbf{a})_{j j}$. Equation (2.122) shows that generically coherences decay to zero with damped oscillations.

To conclude, we have seen that the Redfield equation couples the equations for the populations and the coherences. Hence, it should give better results for systems where those coherences are important. Instead, the populations and coherences evolve independently under the BMS master equation and the coherences typically decay to zero with damped oscillations.

### 2.5.3 Stationary distribution for the thermal bath

To conclude this section, we study the stationary state $\rho^{\text {st }}$ of an open quantum system described by the BMS master equation that is in contact with a thermal bath at inverse temperature $\beta$. In particular, we want to find the stationary state $\rho^{\text {st }}$ corresponding to this setup. Here, we do not specify the microscopic model for the bath Hamiltonian or the interaction.

We start deriving the so-called Kubo-Martin-Schwinger relation for the bath correlation function, which holds for any bath correlation function of a bath in a Gibbs state $\Phi_{\mathrm{B}}(\mathbf{a})=\pi_{\mathrm{B}}(\beta)$. The Kubo-Martin-Schwinger relation is proved by
evaluating the bath correlation function at the imaginary time $t=-\tau-i \beta$ and yields

$$
\begin{equation*}
C_{\alpha^{\prime} \alpha}(\beta ;-\tau-i \beta)=Z_{\mathrm{B}}(\beta)^{-1} \operatorname{tr}\left[e^{-i H_{\mathrm{B}}(\tau+i \beta)} \delta B_{\alpha^{\prime}} e^{i H_{\mathrm{B}}(\tau+i \beta)} \delta B_{\alpha} e^{-\beta H_{\mathrm{B}}}\right]=C_{\alpha \alpha^{\prime}}(\beta ; \tau) . \tag{2.123}
\end{equation*}
$$

This symmetry of the correlation function is translated into the functions $\gamma_{\alpha \alpha^{\prime}}(\beta ; \omega)$ that enter the BMS master equation. We see that

$$
\begin{equation*}
\gamma_{\alpha^{\prime} \alpha}(\beta ;-\omega)=\lambda^{2} \int_{\mathbb{R}} d \tau C_{\alpha \alpha^{\prime}}(\beta ;-\tau-i \beta) e^{-i \omega \tau}=e^{-\beta \omega} \gamma_{\alpha \alpha^{\prime}}(\beta ; \omega), \tag{2.124}
\end{equation*}
$$

which is easily verified for the particular models in Sec. 2.4.1 and Sec. 2.4.2.
Our aim is to find the stationary state $\rho^{\text {st }}$. Knowing that the coherences $\rho_{i j}$ vanish in the long time limit, we focus on finding the population distribution in the stationary state. The populations obey the classical master equation

$$
\begin{equation*}
\partial_{t} p\left(\varepsilon_{i}\right)=\sum_{j \neq i}\left[w\left(\beta ; \varepsilon_{i} \mid \varepsilon_{j}\right) p\left(\varepsilon_{j}\right)-w\left(\beta ; \varepsilon_{j} \mid \varepsilon_{i}\right) p\left(\varepsilon_{i}\right)\right], \tag{2.125}
\end{equation*}
$$

with the temperature-dependent transition rates

$$
\begin{equation*}
w\left(\beta ; \varepsilon_{i} \mid \varepsilon_{j}\right)=\sum_{\alpha \alpha^{\prime}} \gamma_{\alpha \alpha^{\prime}}\left(\beta ; \omega_{j i}\right) S_{\alpha^{\prime}, i j}\left(S_{\alpha, i j}\right)^{*} . \tag{2.126}
\end{equation*}
$$

To find the stationary distribution, since the stationary state fulfills $\partial_{t} p^{\text {st }}\left(\varepsilon_{i}\right)=0$, we look for solutions of Eq. (2.125) with the LHS equal to zero. It follows that the stationary distribution fulfills

$$
\begin{equation*}
\frac{p^{\mathrm{st}}\left(\varepsilon_{i}\right)}{p^{\mathrm{st}}\left(\varepsilon_{j}\right)}=\frac{w\left(\beta ; \varepsilon_{i} \mid \varepsilon_{j}\right)}{w\left(\beta ; \varepsilon_{j} \mid \varepsilon_{i}\right)}=e^{-\beta\left(\varepsilon_{i}-\varepsilon_{j}\right)}, \tag{2.127}
\end{equation*}
$$

where we have used Eq. (2.124) to compute the ratio of the transition rates. In other words $p^{\text {st }}\left(\varepsilon_{i}\right) \propto \exp \left(-\beta \varepsilon_{i}\right)$; that is, the stationary state $\rho^{\text {st }}$ is the Gibbs state $\pi_{\mathrm{s}}(\beta)=\exp \left(-\beta H_{\mathrm{S}}\right) / Z_{\mathrm{s}}(\beta)$ at the same inverse temperature $\beta$ of the bath.

### 2.5.4 The extension to multiple baths

So far, we have considered that the environment of a quantum system is a single unit in equilibrium. However, this is not always the case in practice. The environment of a quantum system is a very large entity, and can itself have subsystems with different microscopic and macroscopic properties. We use the word 'bath' for each subsystem at equilibrium, and refer to this case as an open quantum system in
contact with multiple baths. For instance, two environment subsystems or baths, which are at different temperatures, can interact locally with the open quantum system. In turns out that the description of such setup is already included in the general derivation of the master equations in Sec. 2.2.2 and 2.2.3, and it is revealed by adding additional structure to the interaction Hamiltonian $H_{\text {int }}$, the bath Hamiltonian $H_{\mathrm{B}}$ and the equilibrium state $\Phi_{\mathrm{B}}(\mathbf{a})$.

Consider that the environment is composed by different baths that, to keep the notation light, we label using the Greek letter $v$. For instance, the Hilbert space of the isolated system is now decomposed as $\mathcal{H}=\mathcal{H}_{S} \bigotimes_{v} \mathcal{H}_{v}$. We assume that each bath $v$ is at local equilibrium and described by the state $\Phi_{v}\left(\mathbf{a}_{v}\right)$, with macroscopic equilibrium parameters $\mathbf{a}_{v}$. Also, we consider that the bath Hamiltonian and the interaction can be decomposed as

$$
\begin{align*}
& H_{\mathrm{B}}=\sum_{v} H_{v},  \tag{2.128}\\
& H_{\mathrm{int}}=\lambda \sum_{v} \sum_{\alpha(v)} S_{\alpha(v)} \otimes B_{\alpha(v)} . \tag{2.129}
\end{align*}
$$

The structure in Eqs. (2.128) and (2.129) assumes that the open quantum system only interacts locally with each environment $v$, and that different environment subsystems $v$ and $v^{\prime}$ do not interact with each other.

Given the above structure for $H_{\mathrm{B}}$ and $H_{\text {int }}$, we could now repeat the derivation of Sec. 2.2.2 and 2.2.3. However, the crucial observation is that the "crossed" terms in the bath correlation functions of different environment subsystems vanish; that is,

$$
\begin{equation*}
\operatorname{tr}\left[\delta \tilde{B}_{\alpha(v)}(\tau)^{\dagger} \delta B_{\alpha^{\prime}\left(v^{\prime}\right)} \Phi_{\mathrm{B}}\left(\left\{\mathbf{a}_{v}\right\}\right)\right]=\delta_{v v^{\prime}} C_{\alpha(v) \alpha^{\prime}\left(v^{\prime}\right)}\left(\mathbf{a}_{v} ; \tau\right) \tag{2.130}
\end{equation*}
$$

Formally, this implies that one can simply "add up" the dissipative structure of each independent subsystem $v$ to obtain the master equation for multiple baths. Or more physically, the dissipative processes induced by different baths occur independently of each other. At the level of the Redfield tetradic introduced in Eq. (2.116), the resulting master equation for multiple baths has the structure

$$
\begin{equation*}
\partial_{t} \rho_{i j}=-i\left(\varepsilon_{i}-\varepsilon_{j}\right) \rho_{i j}+\sum_{v} \sum_{k l} R_{v, i j k l}\left(\mathbf{a}_{v}\right) \rho_{k l}, \tag{2.131}
\end{equation*}
$$

where each Redfield tetradic $R_{v, i j k l}\left(\mathbf{a}_{v}\right)$ is computed as if no other baths were present.

### 2.6 Notions on quantum thermodynamics

We conclude this preliminary chapter by introducing a basic framework to study the thermodynamics of open quantum systems. Quantum thermodynamics aims at finding meaningful definitions for thermodynamic quantities, like internal energy or entropy, such that the laws of thermodynamics arise from an underlying quantum mechanical description. In particular, we focus on the first and second law of thermodynamics, which can be summarized as "the energy of the universe is constant, its entropy tends to a maximum", but shall be discussed in more detail. Our description of quantum thermodynamics is based in a "dynamical viewpoint". Namely, if the state of a physical system $\rho$ evolves following a certain equation of motion, how do the laws of thermodynamics emerge from that evolution?

Classically, thermodynamics is often discussed by a working fluid (an open system) upon which one can perform work and that exchanges heat with the environment (see Fig. 2.1). In the following, we discuss the definition of internal energy, work, entropy, and heat, as well as the resulting first and second law of thermodynamics arising from those definitions, when the working fluid is replaced by a quantum system. In the following, we use serif type style letters; e.g. U, W, Q to denote thermodynamic quantities.

### 2.6.1 Internal energy and work

Consider an isolated physical system whose Hamiltonian is described by a timedependent Hamiltonian $H\left(\xi_{t}\right)$. The parameter $\xi_{t}$ is a time-dependent parameter that specifies the driving protocol. For instance, classically, $\xi_{t}$ can parametrize the force exerted to a piston that controls the volume of a container of an ideal gas of particles or, in the quantum regime, $\xi_{t}$ can represent a laser field that exchanges energy with an isolated system. Then, this artificial time-dependence arises as a result of a semi-classical treatment of certain degrees of freedom; for instance, the electromagnetic field. We define the internal energy $\mathrm{U}(t)$ at a time $t$ of a system in the state $\rho(t)$ as the average energy

$$
\begin{equation*}
\mathrm{U}(t):=\operatorname{tr}\left[H\left(\xi_{t}\right) \rho(t)\right] . \tag{2.132}
\end{equation*}
$$

The first law of thermodynamics dictates that the change of internal energy of an isolated system is exclusively due to work. Hence, for consistency, we define

$$
\begin{equation*}
\mathrm{W}(t):=\Delta \mathrm{U}(t)=\operatorname{tr}\left[H\left(\xi_{t}\right) \rho(t)\right]-\operatorname{tr}\left[H\left(\xi_{0}\right) \rho(0)\right] \tag{2.133}
\end{equation*}
$$



Figure 2.1: A classical open system that consists in a working substance (blue circles) is found at equilibrium with its environment. A time-dependent force $F\left(\xi_{t}\right)$ is exerted into the system giving rise to an amount of work $d \mathrm{~W}(t)$ being injected into the working substance. Subsequently, the system reaches the new equilibrium by releasing an amount of heat $d \mathrm{Q}(t)$ to the environment.
where the notation $\Delta$ has been introduced to denote a change in a state function; for instance, $\Delta \mathrm{U}(t):=\mathrm{U}(t)-\mathrm{U}(0)$. Equation (2.133) can be written in the alternative form

$$
\begin{align*}
\mathrm{W}(t) & =\int_{0}^{t} d t^{\prime}\left(\operatorname{tr}\left\{\left[\partial_{t^{\prime}} H\left(\xi_{t^{\prime}}\right)\right] \rho\left(t^{\prime}\right)\right\}+\operatorname{tr}\left\{H\left(\xi_{t^{\prime}}\right)\left[\partial_{t^{\prime}} \rho\left(t^{\prime}\right)\right]\right\}\right) \\
& =\int_{0}^{t} d t^{\prime} \operatorname{tr}\left\{\left[\partial_{t^{\prime}} H\left(\xi_{t^{\prime}}\right)\right] \rho\left(t^{\prime}\right)\right\}=: \int_{0}^{t} d t^{\prime} \dot{\mathrm{W}}\left(t^{\prime}\right), \tag{2.134}
\end{align*}
$$

where the second term in the first line vanishes upon the use of the Liouville-von Neumann equation. Sometimes, we also use the notation $d \mathrm{~W}(t):=\dot{\mathrm{W}}(t) d t$ to refer to the infinitesimal amount of work performed at time $t$.

We assume that the time-dependent driving enters only the system Hamiltonian, in such a way that $H\left(\xi_{t}\right)=H_{\mathrm{S}}\left(\xi_{t}\right)+H_{\mathrm{int}}+H_{\mathrm{B}}$. This is physically justified if we assume that one has only control over the system and not the environment. Then, Eq. (2.134) can be written as

$$
\begin{equation*}
\mathrm{W}(t)=\int_{0}^{t} d t^{\prime} \operatorname{tr}\left\{\left[\partial_{t^{\prime}} H_{\mathrm{S}}\left(\xi_{t^{\prime}}\right)\right] \rho_{\mathrm{S}}\left(t^{\prime}\right)\right\} \tag{2.135}
\end{equation*}
$$

which requires knowledge about only of system quantities; that is, the system Hamiltonian $H_{\mathrm{S}}\left(\xi_{t}\right)$ and the reduced state of the system $\rho_{\mathrm{S}}(t)$. In some experiments, however, the interaction with the bath is turned on and off during the experiment, leading also to a time-dependent interaction $H_{\text {int }}\left(\xi_{t}\right)$. In this scenario one cannot use Eq. (2.135) and has to get back to the original formula in Eq. (2.134).

### 2.6.2 Microscopic candidates for the entropy

One of the central concepts in thermodynamics is entropy. Historically, the thermodynamic entropy $S$ was introduced by Clausius in 1865 [Cla65], and he proposed to call the quantity $S$ entropy, from the Greek $\varepsilon \dot{\varepsilon} v \rho \circ \pi \eta \dot{\eta}$, which means the "transformation content". In the same way that the expectation value of the Hamiltonian gives rise to a microscopic notion of the internal energy of a system, it is of central importance to quantum thermodynamics to give a microscopic definition of the thermodynamic entropy. It turns out that there is not a single candidate for thermodynamic entropy S.

The first notion of microscopic entropy that we discuss is the von Neumann entropy. For a system in an arbitrary state $\rho$, its von Neumann entropy takes the form

$$
\begin{equation*}
\mathrm{S}_{\mathrm{vN}}[\rho]:=-\operatorname{tr}(\rho \log \rho)=-\sum_{i} r_{i} \log r_{i}, \tag{2.136}
\end{equation*}
$$

where $r_{i}$ are the eigenvalues of $\rho$. For a "classical" state $\rho=\sum_{y} p(y)|y \times y|$ with respect to a measurement $Y=\sum_{y} y|y X y|$ of interest, the von Neumann entropy corresponds to the "classical" Shannon entropy

$$
\begin{equation*}
\mathrm{S}_{\mathrm{Sh}}[p(y)]=-\sum_{y} p(y) \log p(y) \tag{2.137}
\end{equation*}
$$

The von Neumann entropy is extensively used in many areas of physics, including quantum information and quantum communication theory, providing a plethora of important results. In quantum thermodynamics, the von Neumann entropy $S_{\mathrm{vN}}$ is a good candidate for the thermodynamic entropy when the system is found in the equilibrium Gibbs state $\pi(\beta)$, that we have already encountered in Sec. 2.4. Also, there is the consensus that it describes correctly the thermodynamic entropy of small open quantum systems that are in weak coupling with a large thermal bath (see Ref. [SW21] and references therein for an extended discussion).

However, the von Neumann entropy $S_{\mathrm{vN}}$ is invariant under unitary evolution, which would imply that the thermodynamic entropy of any isolated system remains constant over time. Then, taking the von Neumann entropy as the thermodynamic entropy goes against the empirical observation that isolated systems tend to increase their entropy over time. Moreover, as it was already acknowledged by von Neumann himself, it is not a good candidate for the macroscopic thermodynamic entropy in general. In the words of von Neumann [Neu10], the von Neumann entropy is "computed from the perspective of an observer who can carry out all measurements that are possible in principle - i.e., regardless of whether they are macroscopic (for example, there every pure state has entropy 0 , only mixtures have entropies greater than 0 !)." Hence, while being useful for small systems, the von Neumann entropy seems too fine-grained to describe the thermodynamic entropy.

A second candidate for the microscopic entropy is the so-called BoltzmannPlanck entropy $S_{B P}$, inspired by the work of Boltzmann [Bol77] but explicitly written down first by Planck[Pla01], which, as a side remark, lies at the heart of the resolution of the ultraviolet catastrophe and the start of the quantum revolution. The Boltzmann-Planck entropy is defined as the logarithm of the number of microstates compatible with a given macroscopic constraint times the Boltzmann constant $k_{\mathrm{B}}$ (hereafter set to $k_{\mathrm{B}}=1$ ). For clarity, let $Y=\sum_{y} y|y \times y|$ be an observable of a large many-body system (for instance the Hamiltonian). For such a large many-body system, the spacing between neighboring outcomes $y$ is potentially very small and resolving each of them becomes practically impossible. Consider that we can only resolve the outcomes $y$ with a resolution $\delta Y$ so that the possible outcomes of the measurement are the coarse-grained values $Y_{x}=x \delta Y$ and $x \in \mathbb{Z}$. To each outcome, we associate the coarse-grained projector $\Pi\left(Y_{x}\right)=\sum_{y} 1_{Y_{x}}(y)|y \times y|$, being $1_{Y_{x}}(y)$ the
indicator function which fulfills

$$
1_{Y_{x}}(y)=\left\{\begin{array}{lc}
1 & \text { if } y \in\left[Y_{x}-\delta Y / 2, Y_{x}+\delta Y / 2\right)  \tag{2.138}\\
0 & \text { else }
\end{array}\right.
$$

Effectively, this finite-resolution measurement corresponds to measuring the coarsegrained observable $\{Y\}=\sum_{x} Y_{x} \Pi\left(Y_{x}\right)$. Then, the outcome $Y_{x}$ is a macroscopic constraint which is compatible with the microstates $y$ such that $1_{Y_{x}}(y)=1$. The number of microscopic states (or volume) compatible with the macroscopic constraint $Y_{x}$ is therefore $v\left(Y_{x}\right)=\operatorname{tr}\left[\Pi\left(Y_{x}\right)\right]$. Hence, according to Boltzmann, we should associate the entropy $\left(k_{\mathrm{B}}=1\right)$

$$
\begin{equation*}
\mathrm{S}_{\mathrm{BP}}\left(Y_{x}\right)=\log v\left(Y_{x}\right), \tag{2.139}
\end{equation*}
$$

to any state which is compatible with $Y_{x}$.
Importantly, the Boltzmann-Planck entropy $\mathrm{S}_{\mathrm{BP}}$ treats equally any state compatible with the macroscopic constraint. Then, if the only information available about the system is that it is constrained to $Y_{x}$, it is reasonable to think that all microstates $y$ compatible with the constraint $Y_{x}$ are equally probable. In this case, the state of the system is described by the microcanonical state

$$
\begin{equation*}
\omega\left(Y_{x}\right):=\frac{\Pi\left(Y_{x}\right)}{v\left(Y_{x}\right)} . \tag{2.140}
\end{equation*}
$$

Interestingly, for the microcanonical state $\omega\left(Y_{x}\right)$ one finds $\mathrm{S}_{\mathrm{vN}}\left[\omega_{\mathrm{B}}\left(E_{x}\right)\right]=\log v\left(E_{x}\right)=$ $\mathrm{S}_{\mathrm{BP}}\left(E_{x}\right)$.

Also, the Boltzmann-Planck entropy allows for an intuitive explanation of the second law. For an isolated system, it is more probable to migrate from regions of small volume to regions of larger volume and reside on the latter for longer times, which is identified as having reached thermodynamic equilibrium. However, the Boltzmann-Planck entropy does not depend on the state of the system, and therefore it seems unable to capture its microscopic dynamics. Also, it seems too subjective. Two different observers with different measurement resolutions $\delta Y$ would predict a different entropy values, with the extreme case that an observer who could resolve all the microscopic details of the many-body system would always find the Boltzmann-Planck entropy equals to zero.

In a sense, the von Neumann entropy is a too fine-grained candidate for the thermodynamic entropy, while the Boltzmann-Planck entropy is too coarse-grained to include any microscopic information. We consider also a third candidate for the microscopic notion of entropy, which will be crucial to our work: the observational entropy. The observational entropy has gained attention recently (see [ŠAS+20] for
a short review), although its use in quantum mechanics can be traced back to the correspondence between Wigner and von Neumann [Neu10]. For a coarse-grained observable $\{Y\}$, the observational entropy is given by

$$
\begin{equation*}
S_{\mathrm{obs}}^{\{Y\}}[\rho]=\sum_{x} p\left(Y_{x}\right)\left[-\log p\left(Y_{x}\right)+\log v\left(Y_{x}\right)\right] . \tag{2.141}
\end{equation*}
$$

where $p\left(Y_{x}\right)$ are the coarse-grained probabilities $\Pi\left(Y_{x}\right)=\operatorname{tr}\left[\rho \Pi\left(Y_{x}\right)\right]$. The observational entropy interpolates nicely between the von Neumann and Boltzmann-Planck entropies in the following sense. Consider an observer who can perform any possible measurement. On the one hand, he could measure $\rho$ exactly, for which we find $\mathrm{S}_{\mathrm{obs}}^{\rho}[\rho]=\mathrm{S}_{\mathrm{vN}}[\rho]$. Also, for any state of the form

$$
\begin{equation*}
\rho=\sum_{x} p\left(Y_{x}\right) \omega\left(Y_{x}\right), \tag{2.142}
\end{equation*}
$$

we find that $S_{\mathrm{obs}}^{\{Y\}}[\rho]=\mathrm{S}_{\mathrm{vN}}[\rho]$. On the other hand, if we know that $\rho$ fulfills the macroscopic constraint; that is, $p\left(Y_{x^{\prime}}\right)=\delta_{x x^{\prime}}$, we find that the observational entropy corresponds to $\mathrm{S}_{\mathrm{obs}}^{\{Y\}}[\rho]=\mathrm{S}_{\mathrm{BP}}\left(Y_{x}\right)$. In general, Eq. (2.141) can be rewritten as

$$
\begin{equation*}
\mathrm{S}_{\mathrm{obs}}^{\{Y\}}[\rho]=\mathrm{S}_{\mathrm{Sh}}\left[p\left(Y_{x}\right)\right]+\sum_{x} p\left(Y_{x}\right) \mathrm{S}_{\mathrm{BP}}\left(Y_{x}\right), \tag{2.143}
\end{equation*}
$$

which reveals that the observational entropy can be rewritten as the Shannon entropy of the distribution $p\left(Y_{x}\right)$ plus the averaged Boltzmann-Planck entropy over the same distribution $p\left(Y_{x}\right)$.

### 2.6.3 The first and second law for open systems

For this subsection, we consider that the isolated system is composed by the open quantum system and the bath. As usual, we decompose the total Hamiltonian as $H=H_{\mathrm{S}}\left(\xi_{t}\right)+H_{\text {int }}\left(\xi_{t}\right)+H_{\mathrm{B}}$. Initially, the state is given by $\rho(0)=\rho_{\mathrm{S}}(0) \otimes \pi_{\mathrm{B}}(\beta)$. Following [ELB10], we take the von Neumann entropy as the thermodynamic entropy for this setup. Moreover, we introduce the reduced system and bath entropies as $\mathrm{S}_{\mathrm{S}}(t)=$ $\mathrm{S}_{\mathrm{vN}}\left[\rho_{\mathrm{S}}(t)\right]=-\operatorname{tr}_{\mathrm{S}}\left[\rho_{\mathrm{S}}(t) \log \rho_{\mathrm{S}}(t)\right]$ and $\mathrm{S}_{\mathrm{B}}(t)=\mathrm{S}_{\mathrm{vN}}\left[\rho_{\mathrm{B}}(t)\right]=-\operatorname{tr}_{\mathrm{B}}\left[\rho_{\mathrm{B}}(t) \log \rho_{\mathrm{B}}(t)\right]$, respectively. Because the von Neumann entropy is preserved under unitary evolution we note

$$
\begin{equation*}
\mathrm{S}(t)=\mathrm{S}(0)=\mathrm{S}_{\mathrm{S}}(0)+\mathrm{S}_{\mathrm{S}}(0) \tag{2.144}
\end{equation*}
$$

Then, we rewrite the change in system entropy as

$$
\begin{align*}
\Delta \mathrm{S}_{\mathrm{S}}(t) & =\mathrm{S}_{\mathrm{S}}(t)-\mathrm{S}(t)+\mathrm{S}_{\mathrm{BP}}(0) \\
& =D\left[\rho(t) \| \rho_{\mathrm{S}}(t) \otimes \pi(\beta)\right]+\operatorname{tr}_{\mathrm{B}}\left\{\left[\rho_{\mathrm{B}}(t)-\pi(\beta)\right] \log \pi(\beta)\right\}, \tag{2.145}
\end{align*}
$$

where we have introduced the always positive relative entropy

$$
\begin{equation*}
D(\rho \| \sigma):=\operatorname{tr}[\rho(\log \rho-\log \sigma)] \geq 0 \tag{2.146}
\end{equation*}
$$

The change in system entropy in Eq. (2.145) has two terms. The first one is always positive, and we identify it with the entropy production $\Sigma$. The second one can be rewritten as

$$
\begin{equation*}
\operatorname{tr}_{\mathrm{B}}\left\{\left[\rho_{\mathrm{B}}(t)-\pi(\beta)\right] \log \pi(\beta)\right\}=-\beta \Delta \mathrm{U}_{\mathrm{B}}(t), \tag{2.147}
\end{equation*}
$$

where $\mathrm{U}(t)=\operatorname{tr}_{\mathrm{B}}\left[H_{\mathrm{B}} \rho_{\mathrm{B}}(t)\right]$ is the internal energy of the bath. Hence, we arrive at the equation

$$
\begin{equation*}
\Delta \mathrm{S}_{\mathrm{S}}(t)+\beta \Delta \mathrm{U}_{\mathrm{B}}(t) \geq 0 \tag{2.148}
\end{equation*}
$$

Equation (2.148) suggests identifying the heat flux $\mathrm{Q}(t)$ as minus the change in bath internal energy; that is, $\mathrm{Q}(t)=:=-\Delta \mathrm{U}_{\mathrm{B}}(t)$. Then, Eq. (2.148) takes the form of the well-known Clausius inequality, which is equivalent to the second law of thermodynamics in the limit of an infinite an ideal heat bath.

Finally, we can connect the definition of the heat current with the first law. We start from the definition of the heat current and note that

$$
\begin{equation*}
\mathrm{Q}(t)=\int_{0}^{t} d t^{\prime} \operatorname{tr}\left[H_{\mathrm{B}} \partial_{t} \rho(t)\right]=\int_{0}^{t} d t^{\prime} \operatorname{tr}\left\{\left[H_{\mathrm{S}}\left(\xi_{t^{\prime}}\right)+H_{\mathrm{int}}\left(\xi_{t^{\prime}}\right)\right] \partial_{t^{\prime}} \rho\left(t^{\prime}\right)\right\} . \tag{2.149}
\end{equation*}
$$

Moreover, from the definition of work in Eq. (2.134), we have

$$
\begin{equation*}
\mathrm{W}(t)=\int_{0}^{t} d t^{\prime} \operatorname{tr}\left\{\partial_{t^{\prime}}\left[H_{\mathrm{S}}\left(\xi_{t^{\prime}}\right)+H_{\mathrm{int}}\left(\xi_{t^{\prime}}\right)\right] \rho\left(t^{\prime}\right)\right\} . \tag{2.150}
\end{equation*}
$$

Hence, if one defines the internal energy of the system as

$$
\begin{equation*}
\mathrm{U}_{\mathrm{S}}(t):=\operatorname{tr}\left\{\left[H_{\mathrm{S}}\left(\xi_{t}\right)+H_{\mathrm{int}}\left(\xi_{t}\right)\right] \rho(t)\right\} \tag{2.151}
\end{equation*}
$$

it follows that

$$
\begin{equation*}
\Delta \mathrm{U}_{\mathrm{S}}(t)=\mathrm{Q}(t)+\mathrm{W}(t), \tag{2.152}
\end{equation*}
$$

which is identical to the first law of thermodynamics.

### 2.7 Chapter's Outlook

In this chapter we have introduced the basic formalism of quantum mechanics, upon which open quantum systems' theory is based. In particular, we have introduced quantum master equations and discussed the Pauli, Redfield and Born-Markovsecular master equations. Then, we have introduced the Nakajima-Zwanzig theory as a general starting point to derive quantum master equations, and we have applied such theory to (re-)obtain the aforementioned master equations of Pauli and Redfield. Then, we have computed the dissipation rates for the infinite non-interacting bosonic and spin heat baths, which will become important in the upcoming chapters. Afterwards, we have reviewed some general properties of quantum master equations like the contractivity of the evolution or the existence of a stationary state. Finally, we have discussed the conventional thermodynamic framework that is used to describe energy and entropy exchanged in open quantum systems.

In the next chapter, we move beyond the infinite bath paradigm and derive a master equation to describe the dynamics of an open quantum system in contact with a finite and dynamically evolving bath.

## Open quantum systems beyond the infinite bath paradigm

In this chapter we study how to describe the evolution of open quantum systems that interact with finite baths, which is one of the central themes of this dissertation. In particular, we define what a finite bath is, and discuss why we expect it to evolve dynamically. Then, we derive the extended microcanonical master equation, a weakcoupling master equation that includes, at a coarse-grained level, a dynamically evolving bath. Afterwards, we consider a model Hamiltonian, which can be solved exactly, to benchmark the dynamics predicted by the extended microcanonical master equation against the Born-Markov-secular master equation and the exact dynamics. Once we are confident that our equation is meaningful, we move to study its general properties, from which we highlight the global energy conservation and the form of the stationary state.

While in some cases, the finiteness and the dynamical nature of the bath are crucial to understand the dynamics, in the appropriate limit we expect our master equation to reduce to the Born-Markov-secular master equation. We formalize this idea and find a Born-Markov-secular master equation at a time-dependent temperature, which interpolates between the extended microcanonical master equation and the Born-Markov-secular master equation (at fixed temperature). Those different approaches can be regarded as a hierarchy of master equations, that
give a more accurate description by including more dynamical bath information. Finally, we compare the dynamics predicted by the hierarchy of equations in the model of a non-interacting spin bath, and study the difference between the three predictions as a function of the relative system size. The results presented in this chapter are largely based on the publications [RSS21b] and [RSS21a].

### 3.1 What are finite baths?

In Chapter 2 we have seen that open quantum systems interact with their environment by exchanging energy and building up system-environment correlations. Very large environments, as compared to the size of the open system, often cause the open system to relax to equilibrium while they keep their macroscopic properties unchanged. We used explicitly this fact in Sec. 2.2.2 to derive the Redfield equation under the name of the Born approximation. Since the influence of the open system on the environment is imperceptible, those environments act as infinite baths. However, not all baths are infinite. In some scenarios, the interaction with the system induces a dynamical evolution of the state of the environment. In turn, the evolution of the environment state has a repercussion on the open system dynamics. In other words, the dynamics of the system and the environment mutually influence each other. Such environments are the central object of study of this work. Since a finite influence from the system can produce a not negligible change in their state, we refer to them as finite baths.

The miniaturization of quantum experiments towards the microscopic scale is leading also to a more detailed description of their surroundings [BMS+12; BGM+13; MLS+15; PSG16; HCS+16; MCL19; KBS+20; HFM+21]. As a consequence, there is often more information available about the bath and, in the case of finite baths, this information evolves dynamically. To date, see for instance [VA17; WKO21], most theoretical and numerical tools to describe the evolution of open quantum systems rely on completely tracing out the environment. However, this modus operandi ignores the dynamical nature of the bath, which could be potentially used to obtain more accurate predictions about the open system dynamics. It is then timely to investigate novel theoretical techniques which profit from this dynamical information by including, to some extent, a dynamically evolving bath.

It is clear that finite baths have to be, at least to some extent, treated dynamically. However, how does one approach, from a theoretical point of view, the dynamics of an open quantum system in contact with a dynamically evolving finite bath? In the following section, we exploit the Nakajima-Zwanzig theory to derive a quantum master equation for dynamically evolving baths.


Figure 3.1: Sketch of the system (labeled by S) interacting with the finite bath (labeled by B). The bath energy levels are depicted with horizontal black lines, and their corresponding energy distribution $p\left(e_{k}\right)$ is plotted in the red solid line. The measurement apparatus (labeled by M) gives an output $E$ given an input $e_{k}$ according to the weighting function $W\left(E \mid e_{k}\right)$, which introduces a finite precision of order $\delta E$.

### 3.2 Dynamically evolving baths

In this section we study how to describe, from a theoretical point of view, the dynamics of an open quantum system that interacts with a dynamically evolving bath. On the one hand, as it is always the case, we are interested in the reduced system dynamics and, therefore, in the evolution of the reduced state of the system $\rho_{\mathrm{S}}=\operatorname{tr}_{\mathrm{B}}(\rho)$. On the other hand, we would like to track the dynamics of the relevant bath variables. The latter can be encoded into one or several bath observables whose evolution influences and is influenced by the open system dynamics. The extraction of the bath dynamical information is done via a quantum measurement of the bath, which can be either projective $\{x, \Pi(x)\}$ or a POVM $\{x, P(x)\}$. Consider, for simplicity, the case of a projective measurement. Then, the bath dynamical information is contained in the evolution of the probabilities $p(x):=\operatorname{tr}[\Pi(x) \rho]$.

Consider the extended state $\rho_{\mathrm{S}}(x)=\operatorname{tr}_{\mathrm{B}}[\Pi(x) \rho]$, which is not normalized. It is clear that, both, the probabilities $p(x)=\operatorname{tr}\left[\rho_{\mathrm{s}}(x)\right]$, and the reduced state of the system $\rho_{\mathrm{S}}=\sum_{x} \rho_{\mathrm{S}}(x)$ can be obtained from $\rho_{\mathrm{S}}(x)$. Thus, we need an equation of motion for the extended state $\rho_{\mathrm{S}}(x)$. In the following subsections, we discuss the case of a projective or a POVM measurement separately.

### 3.2.1 Projective measurements

In Chapter 2, we have seen that the Nakajima-Zwanzig theory is a very versatile tool to describe the evolution of open quantum systems. However, physicists have to choose wisely the relevant map $\mathcal{P}$ to be able to extract the desired dynamical information from the system-bath state $\rho(t)$. We also know that, when the relevant map $\mathcal{P}$ is a projector; that is, $\mathcal{P}^{2}=\mathcal{P}$ the Nakajima-Zwanzig becomes simpler, and the initial states $\rho(0)=\mathcal{P}[\rho(0)]$ are such that the inhomogeneous term $I(t)$ (see Eq. (2.68)) vanishes at all times. Hence, we define the relevant map

$$
\begin{equation*}
\mathcal{P}[\circ]:=\sum_{x} \operatorname{tr}_{\mathrm{B}}\left[\Pi(x)^{\circ}\right] \otimes \frac{\Pi(x)}{v(x)}, \tag{3.1}
\end{equation*}
$$

where the volume $v(x):=\operatorname{tr}[\Pi(x)]$ is equal to the number of eigenstates of the observable $X_{\mathrm{B}}$ within $\Pi(x)$. Using $\Pi(x) \Pi\left(x^{\prime}\right)=\delta_{x x^{\prime}} \Pi(x)$, it is easily check that $\mathcal{P}^{2}=\mathcal{P}$. According to Sec. 2.6.2, we can identify $\Pi(x) / v(x)$ as the microcanonical state corresponding to the macroscopic parameter $x$.

In principle, we are now ready to use all the Nakajima-Zwanzig machinery of Sec. 2.3 and to derive an equation of motion for the set of states $\rho_{\mathrm{s}}(x)$. It is left to chose which is the relevant observable $X_{\mathrm{B}}$. An obvious choice is to pick the bath Hamiltonian $X_{\mathrm{B}}=H_{\mathrm{B}}=\sum_{k} e_{k}\left|e_{k} \times e_{k}\right|$, since, in the end, the energy is the generator of the time-evolution. The only problem with this choice is that it turns out to be too fine-grained for three reasons. First, the bath is a potentially very-large many-body system with a lot of energy eigenstates. Then, finding an equation of motion for every $\rho_{\mathrm{s}}\left(e_{k}\right)$ can be computationally very costly. Second, even with a powerful machine at our disposal, resolving single eigenstates of a many-body system is experimentally very hard. Often, every energy measurement will have a finite energy resolution $\delta E$. Hence, it is not possible to track the evolution of every energy microstate. Finally, as it turns out, a finite energy resolution leads to simpler equations of motion for $\rho_{\mathrm{S}}(x)$. Hence, it is convenient to reduce the complexity of the problem at hand by grouping energy microstates into energy macrostates in a coarse-graining process.

We introduce the energy macrostates or coarse-grained energies $E_{x}=x \delta E$ for integer $x \in \mathbb{Z}$. Then, we consider the coarse-grained energy observable $\left\{H_{B}\right\}=$ $\sum_{x} E_{x} \Pi\left(E_{x}\right)$, where $\Pi(E)=\sum_{k} 1_{E}\left(e_{k}\right)\left|e_{k} X e_{k}\right|$, and we expect that this coarse-grained behavior is enough to describe the macroscopic properties of the bath. Moreover, as already recognized by Boltzmann, a coarse-graining procedure is crucial to reconcile the underlying reversible quantum mechanical description with the irreversible macroscopic world and permits a simplified dynamical description. The same coarsegraining procedure was also used by von Neumann [Neu10] almost a century ago.

In some physical scenarios, one may have more observables $X_{\mathrm{B}}, Y_{\mathrm{B}}, \cdots$ which are needed to describe the dynamically evolving bath. In an early work of van Kampen [Van54], he provided a procedure to include as many observables as needed, provided that they are slowly evolving. Van Kampen identified that slowly evolving observables are the ones which can be macroscopically described, since their "quantummechanical uncertainties are negligible compared to the experimental inaccuracy." Then, one could define projectors $\Pi(\mathbf{x})$ and probabilities $p(\mathbf{x})$ that include the outcomes $\mathbf{x}=(x, y, \cdots)$ of several slowly evolving observables. Despite this is an intriguing research direction, it is left out of the scope of this dissertation.

Finally, we have to discuss how to choose the coarse-graining scale $\delta E$. This is a subtle issue. In principle, the choice of $\delta E$ is left completely arbitrary, since it is a free parameter of the theory. However, some choices of $\delta E$ are more useful for applications than others. In practice, a lower bound for $\delta E$ is given by the experimental accuracy in the energy measurement. Choosing $\delta E$ smaller than the experimental accuracy is meaningless, since the evolution of the corresponding energy levels cannot be tracked. Moreover, a relatively large $\delta E$ can also simplify the dynamical equations. The reason is that, as we shall see, the energy-dependent bath correlation functions decay only if a sufficient number of energy microstates are included in each energy shell. Hence, a Markovian approximation will be available in that case. At the same time, a more coarsed energy structure; that is, a larger $\delta E$, also leads to "fewer" states $\rho_{\mathrm{s}}\left(E_{x}\right)$. However, a too large $\delta E$ can blur some relevant features of the bath density of states, leading to a poor dynamical description. Hence, $\delta E$ has to be chosen such that the coarse-grained bath spectrum still captures the bath energy structure. Hence, albeit being a measurement property, $\delta E$ has to be chosen according to the corresponding finite bath for practical reasons.

### 3.2.2 Imperfect measurements

Measurements are not always sharp or projective. In some scenarios, the probability of obtaining an outcome $E$ after performing an energy measurement given that the actual state was $\left|e_{k}\right\rangle$ is given by a conditional probability distribution $W\left(E \mid e_{k}\right)$, known as the weighting function, which is positive and normalized. The possible outcomes can be either in a continuous range within a certain region; that is, $E \in\left[E_{\min }, E_{\max }\right]$, or obtained from a discrete set $\left\{E_{x}\right\}$ for $x \in \mathbb{Z}$. The POVM elements are given by $P(E)=\sum_{k} W\left(E \mid e_{k}\right)\left|e_{k} X e_{k}\right|$. The corresponding probability distribution $p(E)=\operatorname{tr}[P(E) \rho]$, has to be positive $p(E) \geq 0$ and normalized, which
corresponds to a normalized weighting function

$$
\begin{align*}
& \int d E W\left(E \mid e_{k}\right)=1,  \tag{3.2}\\
& \sum_{x} W\left(E_{x} \mid e_{k}\right)=1 \tag{3.3}
\end{align*}
$$

for the continuous or discrete case, respectively. The weighting function is assumed to be unbiased; that is,

$$
\begin{align*}
& \int d E W\left(E \mid e_{k}\right) E=e_{k}  \tag{3.4}\\
& \sum_{x} W\left(E_{x} \mid e_{k}\right) E_{x}=e_{k} \tag{3.5}
\end{align*}
$$

and to have a variance

$$
\begin{align*}
& \int d E W\left(E \mid e_{k}\right)\left(E-e_{k}\right)^{2}=\delta E^{2}  \tag{3.6}\\
& \sum_{x} W\left(E_{x} \mid e_{k}\right)\left(E_{x}-e_{k}\right)^{2}=\delta E^{2} \tag{3.7}
\end{align*}
$$

To avoid having duplicate equations, from now on we indicate with an integral, both, the continuous and discrete case. A natural choice for the weighting function is the "Gaussian" weighting function $W_{\mathrm{G}}\left(E \mid e_{k}\right)=(\sqrt{2 \pi} \delta E)^{-1} \exp \left[-\left(E-e_{k}\right)^{2} /\left(2 \delta E^{2}\right)\right]$. Another possible choice, that reduces to the projective measurements discussed in the last section, corresponds to a discrete set of outputs $E_{\mathrm{x}}=x \delta E$ with $x \in \mathbb{Z}$ and the "indicator" weighting function $W_{\mathrm{I}}\left(E \mid e_{k}\right)=1_{E}\left(e_{k}\right)$, which equals one if $e_{k} \in[E-\delta E / 2, E+\delta E / 2)$ and zero otherwise.

In order to use the Nakajima-Zwanzig theory, we have to introduce the corresponding relevant map $\mathcal{P}$ in this case. Analogously to the projective measurement case, we chose

$$
\begin{equation*}
\mathcal{P}[\circ]:=\int d E \operatorname{tr}_{\mathrm{B}}\left[P(E)^{\circ}\right] \otimes \omega_{\mathrm{B}}(E), \tag{3.8}
\end{equation*}
$$

where the microcanonical state $\omega_{\mathrm{B}}(E)=P(E) / v(E)$, and the corresponding volume $v(E)=\operatorname{tr}[P(E)]$. However, this choice leads to a complicated Nakajima-Zwanzig equation since, in general, $\mathcal{P}^{2} \neq \mathcal{P}$ and then initial states of the form $\rho(0)=\mathcal{P}\left[{ }^{\circ}\right]$ no longer make the inhomogeneous term $I(t)$ to vanish for all times. Therefore, for this second case, we will take advantage of a different method that below we call the "Redfield approach" to derive the corresponding master equation.

### 3.3 The extended microcanonical master equation

This section is devoted to derive one of the central objects of this dissertation: the extended microcanonical master equation (EMME). On the one hand, the word "extended" makes reference to the fact that the dynamics happens in an extended system space that includes bath variables, in this case the coarse-grained energy. The word "microcanonical" makes reference to the fact that the state $\rho_{\mathrm{S}}(E)$ is associated with the bath being in the microcanonical state $\omega_{B}(E)$. This equation describes the evolution of an open quantum system ' $S$ ' that interacts with a finite bath ' B '. The Hamiltonian of the system bath composite is of the form $H=H_{\mathrm{S}}+$ $H_{\text {int }}+H_{\mathrm{B}}$ where, as usual, $H_{\mathrm{S}}=\sum_{i} \varepsilon_{i}|i \times i|$ and $H_{\mathrm{B}}=\sum_{k} e_{k}\left|e_{k} X e_{k}\right|$ contain only system and bath degrees of freedom, respectively. Instead, $H_{\text {int }}=\lambda \sum_{\alpha} S_{\alpha} \otimes B_{\alpha}$ contains degrees of freedom of, both, the system and the bath. For simplicity, we assume that only there is only one such $\alpha$; that is, $H_{\text {int }}=\lambda S \otimes B$. The case with multiple summands can be work out using analogous techniques to those of Sec. 2.2. We present two different derivations of this equation. The first one, uses the theory of Nakajima and Zwanzig, with the definition of the relevant map

$$
\begin{equation*}
\mathcal{P}[\circ]=\sum_{x} \operatorname{tr}_{\mathrm{B}}\left[\Pi\left(E_{x}\right)^{\circ}\right] \otimes \omega_{\mathrm{B}}\left(E_{x}\right), \tag{3.9}
\end{equation*}
$$

where $\omega_{\mathrm{B}}\left(E_{x}\right)=\Pi\left(E_{x}\right) / v\left(E_{x}\right)$. The second method goes along the lines of Sec. 2.2. Despite requiring an extra assumption, the advantage of the second method is that it is easily generalized to imperfect measurements and, moreover, it is equivalent to the Nakajima-Zwanzig equation within second order in the coupling strength.

Before proceeding, we remark that similar master equations have been found using similar methods than the ones displayed here in the references [EG03; Bud06; BGM06; EG07; Bre07; FB07].

### 3.3.1 The EMME: Nakajima-Zwanzig approach

The starting point of this first approach is the Nakajima-Zwanzig equation (2.67) with the "projective" relevant map $\mathcal{P}$ in Eq. (3.9). For simplicity, we take the initial state $\rho(0)$ to be invariant under the relevant map $\mathcal{P}$; that is, $\rho(0)=\sum_{x} \rho_{\mathrm{S}}\left(E_{x} ; 0\right) \otimes$ $\omega_{\mathrm{B}}\left(E_{x}\right)$, which implies that the inhomogeneous term vanishes $I(t)=0$ for all times $t$.

We start by decomposing the interaction $H_{\text {int }}$ into block-diagonal and blockoffdiagonal parts as

$$
\begin{equation*}
H_{\mathrm{int}}=\sum_{x} H_{\mathrm{s}}^{\operatorname{mf}}\left(E_{x}\right) \otimes \Pi\left(E_{x}\right)+\lambda V \tag{3.10}
\end{equation*}
$$

where we have implicitly defined the mean-field Hamiltonian $H_{S}^{\operatorname{mf}}\left(E_{x}\right):=\lambda\langle B\rangle_{E_{x}} S$. As we already did in Sec. 2.2, we use the shortcut $\left\langle{ }^{\circ}\right\rangle_{E_{x}}:=\operatorname{tr}_{B}\left[{ }^{\circ} \omega_{B}\left(E_{x}\right)\right]$ for expectation values with respect to equilibrium states, and define $\delta B:=B-\sum_{x}\langle B\rangle_{E_{x}}$.

We proceed by computing the different blocks of the Liouvillian $\mathcal{L}[\circ]=-i[H, \circ]$, which we do by direct calculation. In App. B.1, we prove several identities that help in simplifying the computation. The "relevant" block is found to be

$$
\begin{align*}
\mathcal{P} \mathcal{L P} \rho & =-i \sum_{x x^{\prime}} \operatorname{tr}_{\mathrm{B}}\left\{\Pi\left(E_{x}\right)\left[H, \rho_{\mathrm{S}}\left(E_{x^{\prime}}\right) \otimes \omega_{\mathrm{B}}\left(E_{x^{\prime}}\right)\right]\right\} \otimes \omega_{\mathrm{B}}\left(E_{x}\right) \\
& =-i \sum_{x}\left\{\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}\left(E_{x}\right)\right]+\left[H_{\mathrm{S}}^{\operatorname{mf}}\left(E_{x}\right), \rho_{\mathrm{S}}\left(E_{x}\right)\right]\right\} \otimes \omega_{\mathrm{B}}\left(E_{x}\right) . \tag{3.11}
\end{align*}
$$

To compute the Kernel we also need the off-diagonal blocks

$$
\begin{align*}
& \mathcal{Q L P}[\circ]=-i \lambda \sum_{x}\left[V, \operatorname{tr}_{\mathrm{B}}\left[\Pi\left(E_{x}\right) \circ\right] \otimes \omega_{\mathrm{B}}\left(E_{x}\right)\right],  \tag{3.12}\\
& \mathcal{P} \mathcal{L Q}[\circ]=-i \lambda \sum_{x} \operatorname{tr}_{\mathrm{B}}\left\{\Pi\left(E_{x}\right)[V, \circ]\right\} \otimes \omega_{\mathrm{B}}\left(E_{x}\right), \tag{3.13}
\end{align*}
$$

which leads to

$$
\begin{equation*}
\mathcal{K}(t)=-\sum_{x x^{\prime}} \lambda^{2} \operatorname{tr}_{\mathrm{B}}\left\{\Pi\left(E_{x}\right)\left[V, e^{\mathcal{Q} t}\left[\left[V, \operatorname{tr}_{\mathrm{B}}\left[\Pi\left(E_{x^{\prime}}\right), \circ\right] \omega_{\mathrm{B}}\left(E_{x^{\prime}}\right)\right]\right]\right\} \otimes \omega_{\mathrm{B}}\left(E_{x}\right) .\right. \tag{3.14}
\end{equation*}
$$

In principle, the kernel (3.14) can be used into the Nakajima-Zwanzig equation (2.67) to produce the exact dynamics. We are interested into the weak-coupling limit, which allows for a perturbative expansion of the kernel $\mathcal{K}(t)$ in powers of $\lambda$. Then, to the lowest order $\lambda^{2}$, one can replace $\exp (Q \mathcal{L} t)$ by $\exp \left(\mathcal{L}_{0} t\right)$ in Eq. (3.14). There are several ways to see that this is indeed the case. The shortest is probably by making use of the properties $\mathcal{L}=\mathcal{L}_{0}+\mathcal{O}(\lambda),\left[\mathcal{Q}, \mathcal{L}_{0}\right]=0$, and $\mathcal{Q}^{2}=\mathcal{Q}$. Then, from the Taylor series expansion of the exponential, we obtain

$$
\begin{equation*}
e^{\mathcal{Q} t} \approx e^{\mathcal{Q} \mathcal{L}_{0} t}=\sum_{n=0}^{\infty} \frac{\left(\mathcal{Q} \mathcal{L}_{0} t\right)^{n}}{n!}=\mathcal{Q} \sum_{n=1}^{\infty} \frac{\left(\mathcal{L}_{0} t\right)^{n}}{n!}+\mathcal{I}=\mathcal{Q}\left(e^{\mathcal{L}_{0} t}-\mathcal{I}\right)+\mathcal{I}, \tag{3.15}
\end{equation*}
$$

where we have disregarded terms $\mathcal{O}(\lambda)$. It is only left to notice that $\exp (Q \mathcal{L} t)$ appears in the kernel multiplied from left and right by $\mathcal{Q}$. Hence, multiplying Eq. (3.15) by $\mathcal{Q}$ from the left or the right concludes our proof.

We can now use our second order kernel into the Nakajima-Zwanzig equation. Multiplying by $\Pi\left(E_{x}\right)$ and tracing over the bath yields

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}\left(E_{x}\right)= & -i\left[H_{\mathrm{S}}+H_{\mathrm{S}}^{\operatorname{mf}}\left(E_{x}\right), \rho_{\mathrm{S}}\left(E_{x}\right)\right] \\
& -\lambda^{2} \sum_{x^{\prime}} \int_{0}^{t} d t^{\prime} \operatorname{tr}_{\mathrm{B}}\left\{\Pi\left(E_{x}\right)\left[V,\left[\tilde{V}\left(t^{\prime}-t\right), \rho_{\mathrm{S}}\left(E_{x^{\prime}}\right) \otimes \omega\left(E_{x^{\prime}}\right)\right]\right]\right\}, \tag{3.16}
\end{align*}
$$

## CHAPTER 3. OPEN QUANTUM SYSTEMS BEYOND THE INFINITE BATH

 PARADIGMwhere we have used that $\exp \left[i H_{0}\left(t-t^{\prime}\right)\right] \exp \left(-i H t^{\prime}\right)=\exp \left(i H_{0} t\right)+\mathcal{O}(\lambda)$. Equation (3.16) is the time-local version of the EMME, and it is an exact equation within second order in the coupling strength $\lambda$. Equation (3.16) is now ready to be simplified with the help of the Markov and secular approximations, whose validity has to be assessed for the particular problem at hand.

### 3.3.2 The EMME: Redfield approach

In the case of imperfect measurements, represented by POVM elements $P(E)$, the relevant map is no longer a projector. This largely complicates the derivation of the master equation using the Nakajima-Zwanzig theory. Hence, we use here a different strategy which goes along the lines of the one presented in Sec. 2.2.2. Despite being different derivations, it turns out that the resulting equation is equivalent to the Nakajima-Zwanzig result to second order in the coupling strength, which we discuss in App. B.2.

For technical reasons, we start by introducing a different decomposition of the bath coupling operator $B$. Namely, we decompose it into a diagonal

$$
\begin{equation*}
B^{\mathrm{d}}:=\sum_{k}\left\langle e_{k}\right| B\left|e_{k}\right\rangle\left|e_{k} X e_{k}\right|, \tag{3.17}
\end{equation*}
$$

and an offdiagonal part

$$
\begin{equation*}
\delta B:=B-B^{\mathrm{d}}=B-\sum_{k}\left\langle e_{k}\right| B\left|e_{k}\right\rangle\left|e_{k} \chi e_{k}\right| . \tag{3.18}
\end{equation*}
$$

Accordingly, we decompose the interaction $H_{\mathrm{int}}=H_{\mathrm{int}}^{\mathrm{d}}+\lambda V$, where

$$
\begin{equation*}
H_{\mathrm{int}}^{\mathrm{d}}:=\lambda S \otimes B^{\mathrm{d}} \tag{3.19}
\end{equation*}
$$

and the remaining interaction

$$
\begin{equation*}
\lambda V:=H_{\mathrm{int}}-H_{\mathrm{int}}^{\mathrm{d}}=\lambda S \otimes \delta B . \tag{3.20}
\end{equation*}
$$

We now follow a procedure analogous to that of Sec. 2.2.2. First, we go to the interaction picture with respect to $H-\lambda V$. Second, we self-consistently solve the Liouville-von Neumann equation to arrive at

$$
\begin{equation*}
\partial_{t} \bar{\rho}(t)=-i \lambda[\bar{V}(t), \rho(0)]-\lambda^{2} \int_{0}^{t} d t^{\prime}\left[\bar{V}(t),\left[\bar{V}\left(t^{\prime}\right), \bar{\rho}\left(t^{\prime}\right)\right]\right], \tag{3.21}
\end{equation*}
$$

where the bar indicates operators in the interaction picture with respect to $H-\lambda V$.

We now focus in the weak-coupling limit and assume that $\lambda$ is a small energy scale. Then, it makes sense to expand Eq. (3.21) in powers of $\lambda$. As discussed in Sec. 2.2.2, we are allowed to replace $\bar{\rho}\left(t^{\prime}\right)$ by $\bar{\rho}(t)$ within the integral, since $\left|\bar{\rho}\left(t^{\prime}\right)-\bar{\rho}(t)\right| \sim \mathcal{O}(\lambda)$. Going back to the Schrödinger picture, we arrive at

$$
\begin{equation*}
\partial_{t} \rho=-i[H-\lambda V, \rho]-i \lambda[V, \bar{\rho}(-t)]+\lambda^{2} \int_{0}^{t} d t^{\prime}\left[V,\left[\tilde{V}\left(t^{\prime}-t\right), \rho\right]\right]+\mathcal{O}\left(\lambda^{3}\right), \tag{3.22}
\end{equation*}
$$

where $\tilde{V}(t)$ represents, as usual, operators in the interaction picture of $H_{0}=H_{\mathrm{S}}+H_{\mathrm{B}}$, and we have used that $|\bar{V}(t)-\tilde{V}(t)| \sim \mathcal{O}(\lambda)$. To this point, the derivation is identical to that of the Redfield equation. However, we now multiply by the POVM element $P(E)$ and then take the trace over the bath degrees of freedom to obtain

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}(E)= & -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}(E)\right]-i \lambda \operatorname{tr}_{\mathrm{B}}\left\{P(E)\left[H_{\mathrm{int}}^{\mathrm{d}}, \rho\right]\right\}-i \lambda \operatorname{tr}_{\mathrm{B}}\{P(E)[V, \bar{\rho}(-t)]\} \\
& +\lambda^{2} \int_{0}^{t} d t^{\prime} \operatorname{tr}_{\mathrm{B}}\left\{P(E)\left[V,\left[\tilde{V}\left(t^{\prime}-t\right), \rho\right]\right]\right\} . \tag{3.23}
\end{align*}
$$

Equation (3.23) looks already very similar to Eq. (3.16). To conclude our derivation, we perform now a modified Born approximation. Namely, we assume that initially the global state is of the form $\rho(0)=\int d E \rho_{\mathrm{S}}(E ; 0) \otimes \omega_{\mathrm{B}}(E)$ and, moreover, that we can approximate at all times

$$
\begin{equation*}
\rho(t) \approx \int d E \rho_{\mathrm{s}}(E ; t) \otimes \omega_{\mathrm{B}}(E) . \tag{3.24}
\end{equation*}
$$

The intuition behind this modified Born approximation is the following. At time $t=0$, the state of the environment was diagonal in the bath energy eigenbasis. From the Pauli master equation (see Sec. 2.2.1), we know that it is justified to assume that coherences of many-body systems are washed out after a short time $\tau_{\text {rpa }}$. For a sufficiently small energy resolution $\delta E$, states of the form (3.24) corresponds to very general bath energy distributions and, therefore, the approximation is justified. Importantly, this approximation is less restrictive than the standard Born approximation, since it allows for classical correlations between the open quantum system and the bath. Finally, we use Eq. (3.24) into Eq. (3.23),

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}(E)= & -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}(E)\right]-i \int d E^{\prime}\left[H_{\mathrm{S}}^{\mathrm{mf}}\left(E, E^{\prime}\right), \rho_{\mathrm{S}}\left(E^{\prime}\right)\right] \\
& -\lambda^{2} \int_{0}^{t} d t^{\prime} \int d E^{\prime} \operatorname{tr}_{\mathrm{B}}\left\{P(E)\left[V,\left[\tilde{V}\left(t^{\prime}-t\right), \rho_{\mathrm{S}}\left(E^{\prime}\right) \otimes \omega_{\mathrm{B}}\left(E^{\prime}\right)\right]\right]\right\} . \tag{3.25}
\end{align*}
$$

where we have defined $H_{\mathrm{S}}^{\mathrm{mf}}\left(E, E^{\prime}\right)=\lambda \operatorname{tr}_{\mathrm{B}}\left[P(E) B \omega_{\mathrm{B}}\left(E^{\prime}\right)\right] S$. Equation (3.25) is formally equal to the time-local version of the EMME, but includes imperfect measurements of the bath energy.

To conclude, we note that there are two minor differences between Eq. (3.25) and Eq. (3.16). The first, is that the mean-field Hamiltonian $H_{\mathrm{S}}^{\mathrm{mf}}\left(E, E^{\prime}\right)$ depends on two energy arguments in Eq. (3.25), which results from having non-orthogonal POVM elements $P(E)$. The second, is that the definition of the interaction $V$ is slightly different. In particular, the definition in the present section is a fine-grained version of the one in Sec. 3.3.1. Hence, we expect the difference to be unimportant within the coarse-grained view of the bath energy, which is on a scale $\delta E$.

### 3.3.3 The EMME: Markov and secular approximations

In the last two subsections, we have derived a time-local version of the EMME which is ready for numerical implementation. However, the generator of the dynamics is explicitly time-dependent, which complicates the analytical treatment of the equations. As it happened in Sec. (2.2), we can now perform further approximations that make the equation more tractable from a theoretical point of view, and that are physically justified in certain scenarios, which is the aim of this subsection. Since Eq. (3.16) and Eq. (3.25) are formally equal, we can proceed simultaneously with both equations. In the following, we use for convenience the notation of imperfect measurements; that is, as in Eq. (3.25), since they include projective measurements as a particular case.

The first step is to use the decomposition $\lambda V=\lambda S \otimes \delta B$, and rewrite the trace over the bath B in Eq. (3.25) in terms of bath correlation functions. As it turns out, two different types of correlation functions arise. As a function of $\tau=t-t^{\prime}$, we denote them by

$$
\begin{align*}
& C_{1}\left(E, E^{\prime} ; \tau\right):=\langle\delta \tilde{B}(\tau) P(E) \delta B\rangle_{E^{\prime}}=\operatorname{tr}_{\mathrm{B}}\left[\delta \tilde{B}(\tau) P(E) \delta B \omega_{\mathrm{B}}\left(E^{\prime}\right)\right],  \tag{3.26}\\
& C_{2}\left(E, E^{\prime} ; \tau\right):=\langle P(E) \delta \tilde{B}(\tau) \delta B\rangle_{E^{\prime}}=\operatorname{tr}_{\mathrm{B}}\left[P(E) \delta \tilde{B}(\tau) \delta B \omega_{\mathrm{B}}\left(E^{\prime}\right)\right] . \tag{3.27}
\end{align*}
$$

In the case of projective measurements, only one type of correlation function arises since $C_{2}\left(E_{x}, E_{x^{\prime}} ; \tau\right)=\delta_{x x^{\prime}} \sum_{x^{\prime \prime}} C_{1}\left(E_{x^{\prime \prime}}, E_{x} ; \tau\right)$. With the help of Eqs. (3.26) and (3.27), we cast Eq. (3.25) as

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}(E)= & -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}(E)\right]-i \int d E^{\prime}\left[H_{\mathrm{S}}^{\operatorname{mf}}\left(E, E^{\prime}\right), \rho_{\mathrm{S}}\left(E^{\prime}\right)\right]  \tag{3.28}\\
& +\lambda^{2} \iint_{0}^{t} d E^{\prime} d \tau\left[C_{1}\left(E, E^{\prime} ; \tau\right) \tilde{S}(-\tau) \rho_{\mathrm{S}}\left(E^{\prime}\right) S-C_{2}\left(E, E^{\prime} ; \tau\right) S \tilde{S}(-\tau) \rho_{\mathrm{S}}\left(E^{\prime}\right)+\text { h.c. }\right]
\end{align*}
$$

We can now decompose, according to Eq. (2.51), the system interaction in system eigenfrequencies; that is, as $\tilde{S}(t)=\sum_{\omega} S_{\omega} \exp (-i \omega t)$, which leads to

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}(E)= & -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}(E)\right]-i \int d E^{\prime}\left[H_{\mathrm{S}}^{\mathrm{mf}}\left(E, E^{\prime}\right), \rho_{\mathrm{S}}\left(E^{\prime}\right)\right]  \tag{3.29}\\
& +\lambda^{2} \sum_{\omega} \iint_{0}^{t} d E^{\prime} d \tau e^{i \omega \tau}\left[C_{1}\left(E, E^{\prime} ; \tau\right) S_{\omega} \rho_{\mathrm{S}}\left(E^{\prime}\right) S-C_{2}\left(E, E^{\prime} ; \tau\right) S S_{\omega} \rho_{\mathrm{S}}\left(E^{\prime}\right)+\text { h.c. }\right]
\end{align*}
$$

which is still equivalent to Eq. (3.25). To proceed further, we perform the Markov approximation. We proceed analogously to Sec. 2.2.2. First, we assume that the bath correlation functions decay at a timescale $\tau_{\mathrm{B}}$ much faster than the timescale of the evolution of the system. Then, we restrict ourselves to times $t$ smaller than the Poincaré recurrence time $\tau_{\mathrm{P}}$, which can be very large for a many-body bath. Introducing the operators

$$
\begin{equation*}
\theta_{m}\left(E, E^{\prime}\right):=\lambda^{2} \sum_{\omega} \int_{0}^{\infty} d \tau e^{i \omega \tau} C_{m}\left(E, E^{\prime} ; \tau\right) S_{\omega}, \tag{3.30}
\end{equation*}
$$

for $m=1,2$, we arrive at the Redfield version of the EMME

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{s}}(E)= & -i\left[H_{\mathrm{s}}, \rho_{\mathrm{S}}(E)\right]-i \int d E^{\prime}\left[H_{\mathrm{s}}^{\mathrm{mf}}\left(E, E^{\prime}\right), \rho_{\mathrm{S}}\left(E^{\prime}\right)\right] \\
& +\int d E^{\prime}\left[\theta_{1}\left(E, E^{\prime}\right) \rho_{\mathrm{S}}\left(E^{\prime}\right) S-S \theta_{2}\left(E, E^{\prime}\right) \rho_{\mathrm{s}}\left(E^{\prime}\right)+\text { h.c. }\right] \tag{3.31}
\end{align*}
$$

which are analogous to Eq. (2.53).
To conclude the derivation, it is only left to perform the secular approximation. Along the same lines of Sec. 2.2.3, we first define $\Gamma_{m}\left(E, E^{\prime} ; \omega\right):=\lambda^{2} \int_{0}^{\infty} C_{m}\left(E, E^{\prime} ; \tau\right) e^{i \omega \tau}$ for $m=1,2$. Then, we go to the interaction picture with respect to $H_{0}=H_{\mathrm{S}}+H_{\mathrm{B}}$ and use the expansion of $S=\sum_{\omega} S_{\omega}^{\dagger}$ to arrive at

$$
\begin{align*}
\partial_{t} \tilde{\rho}_{\mathrm{S}}(E ; t)= & -i \lambda \sum_{\omega} \int d E^{\prime} \operatorname{tr}_{\mathrm{B}}\left[P(E) B \omega_{\mathrm{B}}\left(E^{\prime}\right)\right] e^{-i \omega t}\left[S_{\omega}, \tilde{\rho}_{\mathrm{S}}\left(E^{\prime} ; t\right)\right] \\
& +\lambda^{2} \sum_{\omega, \omega^{\prime}} \int d E^{\prime} e^{i\left(\omega^{\prime}-\omega\right) t}\left[\Gamma_{1}\left(E, E^{\prime} ; \omega\right) S_{\omega} \rho_{\mathrm{S}}\left(E^{\prime}\right) S_{\omega^{\prime}}^{\dagger}\right. \\
& \left.-\Gamma_{2}\left(E, E^{\prime} ; \omega\right) S_{\omega^{\prime}}^{\dagger} S_{\omega} \rho_{\mathrm{S}}\left(E^{\prime}\right)+\text { h.c. }\right] . \tag{3.32}
\end{align*}
$$

Next, we select the zero frequency component and move back to the Schrödinger
picture, which yields

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}(E)= & -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}(E)\right]-i \int d E^{\prime}\left[H_{\mathrm{S}, 0}^{\mathrm{mf}}\left(E, E^{\prime}\right)+H_{\mathrm{S}}^{\mathrm{LS}}\left(E, E^{\prime}\right), \rho_{\mathrm{S}}\left(E^{\prime}\right)\right]  \tag{3.33}\\
& +\sum_{\omega} \int d E^{\prime}\left[\gamma_{1}\left(E, E^{\prime} ; \omega\right) S_{\omega} \rho_{\mathrm{S}}\left(E^{\prime}\right) S_{\omega}^{\dagger}-\frac{\gamma_{2}\left(E, E^{\prime} ; \omega\right)}{2}\left\{S_{\omega}^{\dagger} S_{\omega}, \rho_{\mathrm{S}}\left(E^{\prime}\right)\right\}\right]
\end{align*}
$$

where we used the sign function, $\operatorname{sign}(\tau)=\tau /|\tau|$ for $\tau \neq 0$ and $\operatorname{sign}(0)=0$, to define

$$
\begin{align*}
& H_{\mathrm{S}, 0}^{\mathrm{mf}}\left(E, E^{\prime}\right)=\lambda\langle P(E) B\rangle_{E^{\prime}} S_{0},  \tag{3.34}\\
& H_{\mathrm{S}}^{\mathrm{LS}}\left(E, E^{\prime}\right)=\frac{\lambda^{2}}{2 i} \sum_{\omega} \int_{\mathrm{R}} d \tau e^{i \omega \tau} \operatorname{sign}(\tau)\langle P(E) \delta \tilde{B}(\tau) \delta B\rangle_{E^{\prime}} S_{\omega}^{\dagger} S_{\omega},  \tag{3.35}\\
& \gamma_{1}\left(E, E^{\prime} ; \omega\right)=\lambda^{2} \int_{\mathbb{R}} d \tau e^{i \omega \tau}\langle\delta \tilde{B}(\tau) P(E) \delta B\rangle_{E^{\prime}},  \tag{3.36}\\
& \gamma_{2}\left(E, E^{\prime} ; \omega\right)=\lambda^{2} \int_{\mathbb{R}} d \tau e^{i \omega \tau}\langle P(E) \delta \tilde{B}(\tau) \delta B\rangle_{E^{\prime}} . \tag{3.37}
\end{align*}
$$

Equation (3.33) is the EMME and is one of the central results of this dissertation. It is interesting to have at hand also the version with projective measurements; that is, we substitute $P(E)$ by $\Pi(E)$, which yields

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}\left(E_{x}\right)= & -i\left[H_{\mathrm{S}}+H_{\mathrm{S}, 0}^{\mathrm{mf}}\left(E_{x}, E_{x}\right)+H_{\mathrm{S}}^{\mathrm{LS}}\left(E_{x}, E_{x}\right), \rho_{\mathrm{S}}\left(E_{x}\right)\right]  \tag{3.38}\\
& +\sum_{\omega} \sum_{x^{\prime}}\left[\gamma_{1}\left(E_{x}, E_{x^{\prime}} ; \omega\right) S_{\omega} \rho_{\mathrm{S}}\left(E_{x^{\prime}}\right) S_{\omega}^{\dagger}-\frac{\gamma_{1}\left(E_{x^{\prime}}, E_{x} ; \omega\right)}{2}\left\{S_{\omega}^{\dagger} S_{\omega}, \rho_{\mathrm{S}}\left(E_{x}\right)\right\}\right],
\end{align*}
$$

where we have used $\gamma_{2}\left(E_{x}, E_{x^{\prime}} ; \omega\right)=\delta_{x x^{\prime}} \sum_{x^{\prime \prime}} \gamma_{1}\left(E_{x^{\prime \prime}}, E_{x} ; \omega\right)$, valid for projective measurements.

### 3.4 Example: Random Matrix Bath Model

We take now the time to investigate a particular "toy-model", which helps to build the right intuition about the dynamics predicted by the EMME. Such toy-model has the property of being analytically solvable and, at the same time, numerically tractable for relatively large bath dimension. A very similar model was already studied in [BGM06], and the results presented here go along the same lines. Also, an extension of this model was studied in Ref. [RSS21b].

To keep everything as simple as possible, we consider a single spin, the open quantum system, which is microscopically described by the Hamiltonian

$$
\begin{equation*}
H_{S}=\sum_{i= \pm} \varepsilon_{i}|i \nmid i|=\frac{\omega_{0}}{2} \sigma_{0}^{z} \tag{3.39}
\end{equation*}
$$



Figure 3.2: Sketch of our toy-model consisting in a spin-1/2 particle coupled to a bath whose coarse-grained energy spectrum forms two bands of width $\delta E$.
where the subscript 0 is used for system properties. For convenience, we label the system energies as $\varepsilon_{-}=-\omega_{0} / 2$ and $\varepsilon_{+}=\omega_{0} / 2$, and the corresponding transitions can have only two values $\omega_{+-}=-\omega_{-+}=\omega_{0}$. Instead, the bath is a potentially large and complicated system whose microscopic description is not available at a finegrained level. However, we know its coarse properties which are encoded in the coarse-grained bath Hamiltonian

$$
\begin{equation*}
\left\{H_{\mathrm{B}}\right\}=\delta E\left\{-\Pi\left(E_{-}\right)+\Pi\left(E_{+}\right)\right\}, \tag{3.40}
\end{equation*}
$$

which corresponds to two bands of width $\delta E>0$ and centered around the energies $E_{x}=x \delta E$. The volumes $v\left(E_{x}\right)=\operatorname{tr}\left[\Pi\left(E_{x}\right)\right]$ correspond to the number of eigenstates on each energy band. For simplicity, we take $\delta E=\omega_{0} / 2$, in such a way that $E_{ \pm}=\varepsilon_{ \pm}$.

We consider an interaction Hamiltonian of the form $H_{\text {int }}=\lambda S \otimes B$, where we know that the system Hamiltonian has the form $S=\sigma_{0}^{x}$, is such a way that

$$
\begin{equation*}
\tilde{S}(\tau)=S_{\omega_{0}} e^{-i \omega_{0} \tau}+S_{-\omega_{0}} e^{i \omega_{0} \tau}=\sigma_{0}^{-} e^{-i \omega_{0} \tau}+\sigma_{0}^{+} e^{i \omega_{0} \tau}, \tag{3.41}
\end{equation*}
$$

where $\sigma_{0}^{ \pm}=| \pm X \mp|$. Instead, we do not know the fine-grained properties of $B$ and, hence, we take a random matrix model for it. In particular, we consider

$$
\begin{equation*}
B=\sum_{e_{k} \in E_{+}} \sum_{e_{q} \in E_{-}} B_{k q}\left|e_{k} X e_{q}\right|+\text { h.c. } \tag{3.42}
\end{equation*}
$$

to be block off-diagonal. The numbers $B_{k q}=B_{q k}^{*}$ are independent and identically
distributed complex random variables of zero mean and variance one; that is,

$$
\begin{align*}
& \mathbb{E}\left[B_{k q}\right]=0,  \tag{3.43}\\
& \mathbb{E}\left[B_{k q} B_{l m}^{*}\right]=\delta_{k q} \delta_{l m}, \tag{3.44}
\end{align*}
$$

and the notation $\mathbb{E}[\circ]$ stands for the average over the random number realizations. Such a model is sketched in Fig. 3.2.

For this system, we can compute the bath correlation function for a single realization of the bath, which yields

$$
\begin{equation*}
C\left(E_{x}, E_{x^{\prime}} ; \tau\right)=\sum_{k q} 1_{E_{x}}\left(e_{q}\right) 1_{E_{x^{\prime}}}\left(e_{k}\right) \frac{B_{k q} B_{k q}^{*}}{v\left(E_{x^{\prime}}\right)} e^{i\left(e_{k}-q_{q}\right) \tau}, \tag{3.45}
\end{equation*}
$$

which, from Eq. (3.42), is different from zero only if $x=+$ and $x^{\prime}=-$ or $x=-$ and $x^{\prime}=+$.

If the volumes $v\left(E_{+}\right)$and $v\left(E_{-}\right)$are sufficiently large, we expect the value of the correlation function not to depend strongly on the particular realization of the random numbers $B_{k q}$. Hence, it is justified to replace the correlation function by its average value over realizations; that is,

$$
\begin{equation*}
C\left(E_{x}, E_{x^{\prime}} ; \tau\right) \approx \frac{1}{v\left(E_{x^{\prime}}\right)}\left[\sum_{k} 1_{E_{x^{\prime}}}\left(e_{k}\right) e^{i e_{\kappa} \tau}\right]\left[\sum_{q} 1_{E_{x}}\left(e_{q}\right) e^{i e_{q} \tau}\right]^{*} . \tag{3.46}
\end{equation*}
$$

This approximation is widely used in random matrix theory, and it relies on the fact that values that deviate largely from the mean are unlikely for many i.i.d. random variables. In the top-left panel of Fig. 3.3, we compare 20 random realizations with the averaged bath correlation in Eq. (3.46) showing very little deviations.

The current expression of the bath correlation function (3.46) still depends on the fine-grained spectrum of the bath. At this point, we can proceed in two different manners. Either we assume a reasonable bath spectrum; for instance, that the energies $e_{k}$ are evenly spaced within each band, or we approximate the sum by an integral with the help of the density of states $g(e):=\sum_{k} \delta\left(e-e_{k}\right)$. It is instructive to compare both approaches.

In the first approach, we relabel the bath energies according to $e_{k} \mapsto E_{x, k_{x}}:=$ $E_{x}+\left[2 k_{x} / v\left(E_{x}\right)-1\right](\delta E / 2)$, where $x$ labels the energy band and $k_{x}$ is an integer that runs $k_{x}=0,1, \cdots, v\left(E_{x}\right)-1$. Hence, we can take advantage of the geometric series to compute

$$
\begin{equation*}
C\left(E_{x}, E_{x^{\prime}} ; \tau\right)=\frac{e^{i\left(E_{x^{\prime}}-E_{x}\right) \tau}}{v\left(E_{x^{\prime}}\right)} \frac{2-2 \cos (\delta E \tau)}{\left[1-e^{i \delta E \tau / v\left(E_{x}\right)}\right]\left[1-e^{-i \delta E \tau / v\left(E_{x^{\prime}}\right)}\right]} . \tag{3.47}
\end{equation*}
$$



Figure 3.3: (top-left): Comparison between 20 realizations of the bath correlation function with random numbers $B_{k q}$ (gray translucid lines) and the correlation function averaged over the random number distribution (orange solid line); (topright) comparison between the averaged bath correlation function Eq. (3.46) (solid orange line) and its approximation in Eq. (3.48) (blue dashed line); (bottom-left) contributions of the positive (orange solid line) and negative (blue dashed line) frequency terms of the real part of the function $\Gamma\left(E_{+}, E_{-} ; \omega, t\right)$; (bottom-right) Comparison of the probability of finding the open quantum system in the state $|+\rangle$ with four methods: integrating the Schrödinger equation (Exact, solid orange line), using the time-local version of the EMME (TL-EMME, blue dashed line), using the Redfield version of the EMME (RF-EMME, dotted yellow line), and using the BMS master equation (purple dot-dashed line). The initial state of the dynamics is $\rho(0)=|+X+| \otimes \Pi\left(E_{-}\right) / v\left(E_{-}\right)$. In all panels, the parameters are $\omega_{0}=2 \delta E, \lambda=10^{-2} \delta E$, $v\left(E_{-}\right)=100$, and $v\left(E_{+}\right)=200$.

In this form, the periodic nature of the correlation function of this finite bath is clear. However, for a many-body system, we expect the density of states $g\left(E_{x}\right) \approx$ $v\left(E_{x}\right) / \delta E$ to be very large. Hence, for times $\tau \ll g\left(E_{x}\right)$ it is justified to expand the denominator in Eq. (3.47) in a Taylor series leading to

$$
\begin{equation*}
C\left(E_{x}, E_{x^{\prime}} ; \tau\right)=e^{i\left(\left(E_{x^{\prime}}-E_{x}\right) \tau\right.} v\left(E_{x}\right) \frac{\sin ^{2}(\delta E \tau / 2)}{(\delta E \tau / 2)^{2}} . \tag{3.48}
\end{equation*}
$$

This procedure leads to a bath correlation function $C\left(E_{x}, E_{x^{\prime}} ; \tau\right)$ that decays on time and for which the Markov approximation is justified. In the top-right panel of Fig. 3.3, we compare the bath correlation function before and after the Taylor expansion of the denominator, showing a very good agreement. Numerically, we observe the first recurrence of the bath correlation function roughly at $\tau=\tau_{\mathrm{P}} \approx$ $315 \delta E^{-1}$.

In the second approach, we take advantage of the density of states $g(e)$ and assume that is approximately constant within each energy band. In particular, we perform the approximate computation

$$
\begin{equation*}
\sum_{k} 1_{E_{x^{\prime}}}\left(e_{k}\right) e^{i e_{k} \tau}=\int_{E_{x^{\prime}}-\delta E / 2}^{E_{x^{\prime}}+\delta E / 2} \operatorname{deg}(e) e^{i e \tau} \approx g\left(E_{x^{\prime}}\right) e^{i E_{x^{\prime}} \tau}(2 i) \sin (\delta E \tau / 2) . \tag{3.49}
\end{equation*}
$$

The next step is using Eq. (3.49) in Eq. (3.46), together with the relation $v\left(E_{x}\right)=$ $g\left(E_{x}\right) \delta E$. This procedure leads exactly to the same correlation function as in Eq. (3.48). Hence, for times $\tau \ll g\left(E_{x}\right)$ the Markovian approximation holds, and the correlation function for the finite bath can be computed as if the bath was infinite and had a continuous spectrum.

For this toy-model, it is possible to find a closed expression even for the timelocal version of the EMME (3.28). Hence, it is convenient to introduce the notation

$$
\begin{equation*}
\Gamma\left(E_{x}, E_{x^{\prime}} ; \omega, t\right)=\lambda^{2} \int_{0}^{t} C\left(E_{x}, E_{x^{\prime}} ; \tau\right) e^{i \omega \tau} \tag{3.50}
\end{equation*}
$$

which fulfills $\Gamma\left(E_{x}, E_{x^{\prime}} ; \omega\right)=\lim _{t \rightarrow \infty} \Gamma\left(E_{x}, E_{x^{\prime}} ; \omega, t\right)$. There are only four non-vanishing options which, for times $t \ll g\left(E_{x}\right)$, read

$$
\begin{align*}
& \Gamma\left(E_{ \pm}, E_{\mp} ; \pm \omega_{0}, t\right)=\lambda^{2} v\left(E_{x}\right) \int_{0}^{t} d \tau \frac{\sin ^{2}(\delta E \tau / 2)}{(\delta E \tau / 2)^{2}},  \tag{3.51}\\
& \Gamma\left(E_{ \pm}, E_{\mp} ; \mp \omega_{0}, t\right)=\lambda^{2} v\left(E_{x}\right) \int_{0}^{t} d \tau e^{\mp i \delta \delta E \tau} \frac{\sin ^{2}(\delta E \tau / 2)}{(\delta E \tau / 2)^{2}} . \tag{3.52}
\end{align*}
$$

It is clear that the second integral is much smaller than the first one, since it is multiplied by the fast oscillating phase $\exp (\mp i 4 \delta E \tau)$ and, hence, we disregard them.

In the bottom-left panel of Fig. 3.3, we compare the contributions with and without the oscillation phase, showing that the later can be safely neglected, specially at long times.

The next step is to define the function

$$
\begin{equation*}
\zeta(t):=\frac{\delta E}{\pi} \int_{0}^{t} \frac{\sin ^{2}(\delta E \tau / 2)}{(\delta E \tau / 2)^{2}} d \tau \tag{3.53}
\end{equation*}
$$

which fulfills $\zeta(t \rightarrow \infty)=1$, and also the dissipation rates

$$
\begin{equation*}
\gamma\left(E_{ \pm}, E_{\mp} ; \pm \omega_{0}\right)=2 \lim _{t \rightarrow \infty} \int_{0}^{\infty} \Gamma\left(E_{ \pm}, E_{\mp} ; \pm \omega_{0}, t\right)=2 \pi \lambda^{2} \frac{v\left(E_{ \pm}\right)}{\delta E} \tag{3.54}
\end{equation*}
$$

such that $2 \Gamma\left(E_{ \pm}, E_{\mp} ; \pm \omega_{0}, t\right)=\zeta(t) \gamma\left(E_{ \pm}, E_{\mp} ; \pm \omega_{0}\right)$, and the other combinations are set to zero.

Finally, we are ready to write down the time-local version of the EMME for this model. It yields

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}\left(E_{ \pm}\right)= & -i \frac{\omega_{0}}{2}\left[\sigma_{0}^{z}, \rho_{\mathrm{S}}\left(E_{ \pm}\right)\right] \\
& +\frac{\zeta(t)}{2} \frac{2 \pi \lambda^{2}}{\delta E} v\left(E_{ \pm}\right)\left\{\sigma^{\mp} \rho_{\mathrm{S}}\left(E_{\mp}\right) \sigma_{x}-\frac{v\left(E_{\mp}\right)}{v\left(E_{ \pm}\right)}|\mp X \mp| \rho_{\mathrm{S}}\left(E_{ \pm}\right)+\text {h.c. }\right\} \tag{3.55}
\end{align*}
$$

From the time-local equation (3.55), it is easy to obtain the Redfield equation by replacing $\zeta(t) \mapsto 1$ and also the EMME by replacing, additionally, $\sigma_{x} \mapsto \sigma^{\mp}$. Moreover, projecting into the system energy eigenstates we obtain the classical master equation

$$
\begin{align*}
& \partial_{t} p\left(\varepsilon_{ \pm}, E_{ \pm}\right)=0,  \tag{3.56}\\
& \partial_{t} p\left(\varepsilon_{\mp}, E_{ \pm}\right)=\zeta(t) \frac{2 \pi \lambda^{2}}{\delta E}\left[v\left(E_{ \pm}\right) p\left(\varepsilon_{ \pm}, E_{\mp}\right)-v\left(E_{\mp}\right) p\left(\varepsilon_{\mp}, E_{ \pm}\right)\right] . \tag{3.57}
\end{align*}
$$

for the populations $p\left(\varepsilon_{i}, E_{x}\right):=\langle i| \rho_{\mathrm{S}}\left(E_{x}\right)|i\rangle$, which is identical for the Redfield and secular versions of the EMME. Interestingly, it exists a closed form solution for this classical master equation.

To solve the coupled differential equations in Eq. (3.57), we introduce the column probability vector $\mathbf{p}=\left[p\left(\varepsilon_{-}, E_{+}\right), p\left(\varepsilon_{+}, E_{-}\right)\right]^{T}$, where the probabilities $p\left(\varepsilon_{-}, E_{-}\right)$ and $p\left(\varepsilon_{+}, E_{+}\right)$are left out since they do not take part in the dynamics. Then, the differential equations can be cast in matrix form as

$$
\begin{equation*}
\partial_{t} \mathbf{p}=\zeta(t) \Lambda \mathbf{p} \tag{3.58}
\end{equation*}
$$

where we have defined the stochastic dynamical matrix

$$
\Lambda=\frac{2 \pi \lambda^{2}}{\delta E}\left(\begin{array}{cc}
-v\left(E_{-}\right) & v\left(E_{+}\right)  \tag{3.59}\\
v\left(E_{-}\right) & -v\left(E_{+}\right)
\end{array}\right) .
$$

We can now integrate Eq. (3.58) to obtain the full time-dependence of the probability vector

$$
\begin{equation*}
\mathbf{p}(t)=e^{Z(t) \Lambda} \mathbf{p}(0) . \tag{3.60}
\end{equation*}
$$

where $Z(t)=\int_{0}^{t} d t^{\prime} \zeta\left(t^{\prime}\right)$. Finally, we note that the matrix $\Lambda$ has the property

$$
\begin{equation*}
\Lambda^{2}=\frac{2 \pi \lambda^{2}}{\delta E}\left[v\left(E_{-}\right)+v\left(E_{+}\right)\right] \Lambda:=2 \bar{\gamma} \Lambda . \tag{3.61}
\end{equation*}
$$

which leads to the final solution

$$
\begin{equation*}
\mathbf{p}(t)=\sum_{n=0}^{\infty} \frac{[Z(t) \Lambda]^{n}}{n!} \mathbf{p}(0)=\left(\mathbf{1}+\frac{1-e^{-2 \bar{\gamma} Z(t)}}{2 \bar{\gamma}} \Lambda\right) \mathbf{p}(0) \tag{3.62}
\end{equation*}
$$

In the bottom-right panel of Fig. 3.3, we benchmark the dynamics of the probability $p\left(\varepsilon_{+}\right)$obtained with the time-local version of the EMME (blue dashed line) against the exact dynamics (orange solid line), showing almost a perfect agreement. For comparison, we also include the dynamics of $p\left(\varepsilon_{+}\right)$using the Redfield version of the EMME (yellow dotted line), which fails at describing the short-time behavior, but describes correctly the long-time dynamics. Finally, we also include the results of the BMS master equation (purple dot-dashed line), which, for the finite bath at hand, fails to capture the dynamics completely.

Since the function $\zeta(t)$ rapidly saturates to $\zeta(t \rightarrow \infty)=1$, we expect $Z(t) \sim t$ at long times. Therefore, the stationary distribution can be computed

$$
\begin{equation*}
\frac{p^{\mathrm{st}}\left(\varepsilon_{+}, E_{-}\right)}{p^{\mathrm{st}}\left(\varepsilon_{-}, E_{+}\right)}=\frac{v\left(E_{-}\right)}{v\left(E_{+}\right)} . \tag{3.63}
\end{equation*}
$$

The toy-model at hand excels for being particularly simple, and allowing for a closed form solution of the dynamical equations. However, much of the discussion and the intuition of this model can be extrapolated to more general baths. In particular, for strongly non-integrable many-body baths, which are well approximated using random matrix models, most of the discussion should hold. In the following section, we study general properties of the EMME some of which we have encountered for the present random matrix model.

### 3.5 Properties of the EMME

In the last section we have obtained the EMME, a master equation to describe the dynamics of an open quantum system in contact with a finite bath. In this section, we investigate the general properties of this master equation, which will help us to build a physical intuition. To this end, we first explicitly compute the Lamb shift Hamiltonian (3.35), and the dissipation rates (3.36) and (3.37), which help with the discussion. The Lamb shift yields

$$
\begin{equation*}
\left.H_{\mathrm{S}}^{\mathrm{LS}}\left(E, E^{\prime}\right)=\lambda^{2} \sum_{\omega} \sum_{k q} W\left(E \mid e_{q}\right) \frac{W\left(E^{\prime} \mid e_{q}\right)}{v\left(E^{\prime}\right)}\left|\left\langle e_{q}\right| \delta B\right| e_{k}\right\rangle\left.\right|^{2} S_{\omega}^{\dagger} S_{\omega} \mathrm{PV}\left\{\frac{1}{\omega+e_{q}-e_{k}}\right\}, \tag{3.64}
\end{equation*}
$$

where the principal value arises from the Sokhotski-Plemelj theorem (see Sec. 2.4.1). Next, we explicitly write down the dissipation rates

$$
\begin{align*}
& \left.\gamma_{1}\left(E, E^{\prime} ; \omega\right)=2 \pi \lambda^{2} \sum_{k q}\left|\left\langle e_{k}\right| \delta B\right| e_{q}\right\rangle\left.\right|^{2} W\left(E \mid e_{k}\right) \frac{W\left(E^{\prime} \mid e_{q}\right)}{v\left(E^{\prime}\right)} \delta\left(e_{k}-e_{q}-\omega\right),  \tag{3.65}\\
& \left.\gamma_{2}\left(E, E^{\prime} ; \omega\right)=2 \pi \lambda^{2} \sum_{k q}\left|\left\langle e_{k}\right| \delta B\right| e_{q}\right\rangle\left.\right|^{2} W\left(E \mid e_{q}\right) \frac{W\left(E^{\prime} \mid e_{q}\right)}{v\left(E^{\prime}\right)} \delta\left(e_{k}-e_{q}-\omega\right) . \tag{3.66}
\end{align*}
$$

where, again, the $\delta$-functions arise from the Sokhotski-Plemelj theorem. As it happened with the master equations in Sec. 2.2, the principal value and the $\delta$ functions appear as a consequence of the Markov approximation and can only be treated consistently within the infinite bath limit. Instead, we should interpret them as time-independent approximations of the "actual" finite bath dissipation rates for times $t$ smaller than the Poincaré recurrence time $\tau_{\mathrm{P}}$, as we did in Sec. 3.4.

### 3.5.1 Total average energy conservation

The first property we look at is energy conservation. In general, isolated mechanical systems evolve in such a way that their energy is preserved over time. This property should arise at some level for the open quantum system and finite bath composite. Here, we prove that the average energy of system plus finite bath is conserved.

To see that the average energy is conserved, we start defining the system and
bath (internal) energy as

$$
\begin{align*}
& \mathrm{U}_{\mathrm{S}}:=\int d E \operatorname{tr}_{\mathrm{S}}\left[H_{\mathrm{S}} \rho_{\mathrm{S}}(E)\right],  \tag{3.67}\\
& \mathrm{U}_{\mathrm{B}}:=\int d E E \operatorname{tr}_{\mathrm{S}}\left[\rho_{\mathrm{S}}(E)\right], \tag{3.68}
\end{align*}
$$

whose sum $U=U_{S}+U_{B}$ corresponds to the total energy. Then, taking the time derivative of the total energy and rearranging terms, we obtain

$$
\begin{equation*}
\partial_{t} \mathrm{U}=\iint d E d E^{\prime} \sum_{\omega}\left\{E\left[\gamma_{1}\left(E, E^{\prime} ; \omega\right)-\gamma_{2}\left(E, E^{\prime} ; \omega\right)\right]-\omega \gamma_{1}\left(E, E^{\prime} ; \omega\right)\right\} \operatorname{tr}\left[S_{\omega}^{\dagger} S_{\omega} \rho_{\mathrm{S}}\left(E^{\prime}\right)\right] \tag{3.69}
\end{equation*}
$$

where we have used that $\left[H_{\mathrm{S}}, S_{\omega}\right]=-\omega S_{\omega}$. It is only left to use Eq. (3.65) and (3.66) and the fact that the weighting function $W\left(E \mid e_{k}\right)$ is unbiased and normalized to perform the integral over $E$. Then, under the use of the $\delta$-function, brings us to the energy conservation property $\partial_{t} U=0$.

The fact that the dynamics of the EMME preserve the total energy $U=U_{S}+U_{B}$ can be seen as a dynamical constraint that selects the dynamical processes that are possible. For instance, a transition from a lower to a higher energy state of the system has to be accompanied from a higher to lower transition on the bath that supplies the corresponding energy deficit (on average).

### 3.5.2 Population dynamics and the stationary state

In Sec. 2.5.2, we have seen that after the secular approximation the populations $p(i)=\left(\rho_{\mathrm{S}}\right)_{i i}$ and the coherences $\left(\rho_{\mathrm{S}}\right)_{i j}$ evolved autonomously. As show below, this is also the case for the EMME with the caveat that energy populations are a joint distribution of the system and bath energy in the extended space.

We start by introducing the shortcut notation $p\left(\varepsilon_{i}, E\right):=\langle i| \rho_{\mathrm{S}}(E)|i\rangle$ for the energy populations, which corresponds to a joint probability distribution of system and bath energy. Naturally, the reduced probabilities $p\left(\varepsilon_{i}\right)=\int d E p\left(\varepsilon_{i}, E\right)$ and $p(E)=$ $\sum_{i} p\left(\varepsilon_{i}, E\right)$ can be obtained from this joint probability distribution. The dynamics of this object can be obtained by projecting the EMME into the $i^{\text {th }}$ eigenstate, which yields

$$
\begin{equation*}
\left.\partial_{t} p\left(\varepsilon_{i}, E\right)=\sum_{j} \int d E^{\prime}|\langle i| S| j\right\rangle\left.\right|^{2}\left\{\gamma_{1}\left(E, E^{\prime} ; \omega_{j i}\right) p\left(\varepsilon_{j}, E^{\prime}\right)-\gamma_{2}\left(E, E^{\prime} ; \omega_{i j}\right) p\left(\varepsilon_{i}, E^{\prime}\right)\right\}, \tag{3.70}
\end{equation*}
$$

which shows that the joint probabilities $p\left(\varepsilon_{i}, E\right)$ evolve autonomously. Unfortunately, not much more can be said about the evolution of the energy populations for the case of imperfect measurements. Regarding the coherences $\left[\rho_{\mathrm{S}}(E)\right]_{i j}$ with $i \neq j$, with the assumptions of a non-degenerate spectrum with non-degenerate transitions, we find the evolution equation

$$
\begin{align*}
\partial_{t}\left[\rho_{\mathrm{S}}(E)\right]_{i j}= & -i \int d E^{\prime}\left[H_{\mathrm{S}}^{\prime}\left(E, E^{\prime}\right)_{i i}-H_{\mathrm{S}}^{\prime}\left(E, E^{\prime}\right)_{j j}\right]\left[\rho_{\mathrm{S}}\left(E^{\prime}\right)\right]_{i j} \\
& \left.-\sum_{l} \int d E^{\prime}|\langle l| S| i\right\rangle\left.\right|^{2} \gamma_{2}\left(E, E^{\prime} ; \omega_{i l}\right)\left[\rho_{\mathrm{S}}\left(E^{\prime}\right)\right]_{i j}, \tag{3.71}
\end{align*}
$$

which shows that coherences also evolve autonomously.
Instead, the version with projective measurements reveals more physical features about the dynamics. For projective measurements, the Eq. (3.70) simplifies into

$$
\begin{equation*}
\partial_{t} p\left(\varepsilon_{i}, E_{x}\right)=\sum_{j} \sum_{x^{\prime}}\left\{w\left(\varepsilon_{i}, E_{x} \mid \varepsilon_{j}, E_{x^{\prime}}\right) p\left(\varepsilon_{j}, E_{x^{\prime}}\right)-w\left(\varepsilon_{i}, E_{x^{\prime}} \mid \varepsilon_{j}, E_{x}\right) p\left(\varepsilon_{i}, E_{x}\right)\right\}, \tag{3.72}
\end{equation*}
$$

which has the form of a classical master equation (2.21) with the transition rates $\left.w\left(\varepsilon_{i}, E_{x} \mid \varepsilon_{j}, E_{x^{\prime}}\right):=|\langle i| S| j\right\rangle\left.\right|^{2} \gamma_{1}\left(E_{x}, E_{x^{\prime}} ; \varepsilon_{j}-\varepsilon_{i}\right)$. Often, it is convenient to introduce a probability vector $\mathbf{p}$ with components $p\left(\varepsilon_{i}, E_{x}\right)$ and write the evolution equation in the compact matrix form

$$
\begin{equation*}
\partial_{t} \mathbf{p}=\Lambda \mathbf{p} \tag{3.73}
\end{equation*}
$$

where the dynamical matrix $\Lambda$ has components

$$
\begin{equation*}
(\Lambda)_{i j x y}=w\left(\varepsilon_{i}, E_{x} \mid \varepsilon_{j}, E_{x^{\prime}}\right)-\delta_{i j} \delta_{x y} \sum_{i^{\prime} x^{\prime}} w\left(\varepsilon_{i^{\prime}}, E_{x^{\prime}} \mid \varepsilon_{i}, E_{x}\right) . \tag{3.74}
\end{equation*}
$$

The stationary state of Eq. (3.72) is found by imposing that the LHS of Eq. (3.72) vanishes. Then, we find that

$$
\begin{equation*}
\frac{p^{\mathrm{st}}\left(\varepsilon_{i}, E_{x}\right)}{p^{\text {stt}}\left(\varepsilon_{j}, E_{x^{\prime}}\right)}=\frac{w\left(\varepsilon_{i}, E_{x} \mid \varepsilon_{j}, E_{x^{\prime}}\right)}{w\left(\varepsilon_{j}, E_{x^{\prime}} \mid \varepsilon_{i}, E_{x}\right)}=\frac{v\left(E_{x}\right)}{v\left(E_{x^{\prime}}\right)}, \tag{3.75}
\end{equation*}
$$

Physically, the stationary condition in Eq. (3.75) says that the probability of having a system energy $\varepsilon_{i}$ and a macroscopic bath energy $E_{x}$ is proportional to the number of microscopic states $\left|e_{k}\right\rangle$ compatible with that macroscopic energy, which demonstrates once more the microcanonical character of the EMME. Indeed, Eq. (3.75) is the microcanonical counterpart of the canonical stationary condition

Eq. (2.127). This relation is made even more explicit by rewriting Eq. (3.75) in terms of the Boltzmann-Planck entropy $\mathrm{S}_{\mathrm{BP}}(E)=\log [v(E)]$. Then, we find

$$
\begin{equation*}
\frac{p^{\mathrm{st}}\left(\varepsilon_{i}, E_{x}\right)}{p^{\mathrm{st}}\left(\varepsilon_{j}, E_{x^{\prime}}\right)}=e^{\mathrm{S}_{\mathrm{SP}}\left(E_{x}\right)-\mathrm{S}_{\mathrm{BP}}\left(E_{x^{\prime}}\right)} . \tag{3.76}
\end{equation*}
$$

As a final remark, while the probability distribution in Eq. (3.75) is always stationary, but it may not be the only one. In particular, if other quantities are conserved during the evolution, the stationary distribution must be compatible with the initial value of the conserved quantities. In the following subsection, we discuss the case when the conserved quantity is the total energy.

### 3.5.3 Emergent block-structure for the population dynamics

We again restrict ourselves to the case of projective measurements and ask the following question: Does the average energy conservation constraint add any additional structure to the classical master equation for the energy populations (3.72)?

To answer this question, consider the transition rate $w\left(\varepsilon_{i}, E_{x} \mid \varepsilon_{j}, E_{x^{\prime}}\right)$, which explicitly reads

$$
\begin{equation*}
w\left(\varepsilon_{i}, E_{x} \mid \varepsilon_{j}, E_{x^{\prime}}\right)=2 \pi \lambda^{2} \sum_{k q} \frac{\left.\left|\left\langle i, e_{k}\right| V\right| j, e_{q}\right\rangle\left.\right|^{2}}{v\left(E_{x^{\prime}}\right)} 1_{E_{x}}\left(e_{k}\right) 1_{E_{x^{\prime}}}\left(e_{q}\right) \delta\left(e_{k}-e_{q}-\omega_{j i}\right) . \tag{3.77}
\end{equation*}
$$

Now consider that $\delta E$ is chosen in such a way that the approximation

$$
\begin{equation*}
1_{E_{x}}\left(e_{k}\right) 1_{E_{x^{\prime}}}\left(e_{q}\right) \delta\left(e_{k}-e_{q}-\omega_{j i}\right) \approx \delta_{E_{x^{\prime}}, E_{x}+\omega_{i j}}, \tag{3.78}
\end{equation*}
$$

is justified. Then, the classical master equation for the populations turns into

$$
\begin{equation*}
\partial_{t} p\left(\varepsilon_{i}, E_{x}\right)=\sum_{j}\left\{w\left(\varepsilon_{i}, E_{x} \mid \varepsilon_{j}, E_{x^{\prime}}+\omega_{i j}\right) p\left(\varepsilon_{j}, E_{x}+\omega_{i j}\right)-w\left(\varepsilon_{i}, E_{x}+\omega_{i j} \mid \varepsilon_{j}, E_{x}\right) p\left(\varepsilon_{i}, E_{x}\right)\right\}, \tag{3.79}
\end{equation*}
$$

To reveal the block structure, consider the total energy $E_{\text {tot }}=\varepsilon_{i}+E_{x}$ and its corresponding probability distribution $p_{\mathrm{tot}}\left(E_{\mathrm{tot}}\right):=\sum_{i} p\left(\varepsilon_{i}, E_{\mathrm{tot}}-\varepsilon_{i}\right)$. Then, it is clear that

$$
\begin{align*}
\partial_{t} p_{\mathrm{tot}}\left(E_{\mathrm{tot}}\right)= & \sum_{i j}\left\{w\left(\varepsilon_{i}, E_{\mathrm{tot}}-\varepsilon_{i} \mid \varepsilon_{j}, E_{\mathrm{tot}}-\varepsilon_{j}\right) p\left(\varepsilon_{j}, E_{\mathrm{tot}}-\varepsilon_{j}\right)\right. \\
& \left.-w\left(\varepsilon_{j}, E_{\mathrm{tot}}-\varepsilon_{j} \mid \varepsilon_{i}, E_{\mathrm{tot}}-\varepsilon_{i}\right) p\left(\varepsilon_{i}, E_{\mathrm{tot}}-\varepsilon_{i}\right)\right\}=0 \tag{3.80}
\end{align*}
$$

that is, the dynamics breaks into blocks of conserved total energy. Accordingly, the stationary distribution should now "remember" its total energy. Because probabilities belonging to different total energies are disconnected, we have that

$$
\begin{equation*}
\frac{p^{\mathrm{st}}\left(\varepsilon_{i}, E_{\mathrm{tot}}-\varepsilon_{i}\right)}{p^{\mathrm{st}}\left(\varepsilon_{j}, E_{\mathrm{tot}}-\varepsilon_{j}\right)}=\frac{v\left(E_{\mathrm{tot}}-\varepsilon_{i}\right)}{v\left(E_{\mathrm{tot}}-\varepsilon_{j}\right)}, \tag{3.81}
\end{equation*}
$$

Equation (3.81) is less restrictive than the original stationary condition (3.75) since it is only applied to probabilities that belong to the same total energy $E_{\text {tot }}$. If we use the Boltzmann-Planck entropy

$$
\begin{equation*}
\frac{p^{\mathrm{st}}\left(\varepsilon_{i}, E_{\mathrm{tot}}-\varepsilon_{i}\right)}{p^{\mathrm{st}}\left(\varepsilon_{j}, E_{\mathrm{tot}}-\varepsilon_{j}\right)}=e^{\mathrm{S}_{\mathrm{BP}}\left(E_{\mathrm{tot}}-\varepsilon_{i}\right)-\mathrm{S}_{\mathrm{BP}}\left(E_{\mathrm{tot}}-\varepsilon_{j}\right)} \approx e^{-\beta\left(E_{\mathrm{tot}}\right) \omega_{i j}}, \tag{3.82}
\end{equation*}
$$

where $\beta(E):=\partial_{E} \mathrm{~S}_{\mathrm{BP}}(E)$ is the Boltzmann inverse temperature. Hence, the total energy conservation gives rise to an effective thermal distribution provided that $\mathrm{S}_{\mathrm{BP}}(E)$ is a sufficiently slow varying function of $E$.

While the discussion of this subsection provides insights about how energy is conserved during the dynamics, it also requires further approximations. Also, we have swept under the carpet that the coarse-grained bath energy $E_{\text {tot }}-\varepsilon_{i}$ may not be defined. For this reason, we shall return to the general case in the following.

### 3.5.4 System-bath correlations

The standard derivation of master equations that we discussed in Sec. 2.2.2 and 2.2.3 takes advantage of the Born approximation, which assumes that the correlations between the system and the bath are negligible. One of the distinctive features of the EMME is that it is capable of capturing part of the system-bath correlations. Hence, it can be used to assess the validity of the Born approximation.

To quantify the possibly quantum system bath correlations, we introduce the always positive quantum mechanical mutual information

$$
\begin{equation*}
I_{\mathrm{S}: \mathrm{B}}^{\mathrm{qm}}[\rho]:=\mathrm{S}_{\mathrm{vN}}\left[\rho_{\mathrm{S}}\right]+\mathrm{S}_{\mathrm{vN}}\left[\rho_{\mathrm{B}}\right]-\mathrm{S}_{\mathrm{vN}}[\rho] \geq 0 \tag{3.83}
\end{equation*}
$$

which equals zero only if the state is fully decorrelated; that is, if $\rho=\rho_{\mathrm{S}} \otimes \rho_{\mathrm{B}}$. Equivalently, we could have defined $I_{\mathrm{S}: \mathrm{B}}^{\mathrm{qm}}[\rho]$ through the relative entropy as

$$
\begin{equation*}
I_{\mathrm{S}: \mathrm{B}}^{\mathrm{qm}}[\rho]:=D\left(\rho \| \rho_{\mathrm{S}} \otimes \rho_{\mathrm{B}}\right) . \tag{3.84}
\end{equation*}
$$

This mutual information is particularly useful for relatively small quantum systems, whose total state $\rho$ is available.

Instead, the EMME only captures part of the system-bath correlations, namely, those encoded in the joint probability distribution $p\left(\varepsilon_{i}, E\right)$. Those correlations can be quantified by means of the classical mutual information

$$
\begin{equation*}
I_{\mathrm{S}: \mathrm{B}}^{\mathrm{cl}}\left[\left\{p\left(\varepsilon_{i}, E\right)\right\}\right]:=\sum_{i} \int d E p\left(\varepsilon_{i}, E\right)\left[\log p\left(\varepsilon_{i}, E\right)-\log p\left(\varepsilon_{i}\right)-\log p(E)\right] \geq 0 \tag{3.85}
\end{equation*}
$$

In fact, one can see that

$$
\begin{equation*}
I_{\mathrm{S}: \mathrm{B}}^{\mathrm{qm}}(\rho) \geq I_{\mathrm{S}: \mathrm{B}}^{\mathrm{cl}}(\mathbf{p}) \geq 0, \tag{3.86}
\end{equation*}
$$

where the first equality is reached for $\rho=\int d E \sum_{i} p\left(\varepsilon_{i}, E\right)\left|i \chi_{i}\right| \otimes \omega_{\mathrm{B}}(E)$.
Physically speaking, the reason why we can observe strong system-bath correlations with the EMME arises from the fact that the total average energy $U$ is conserved under the evolution, which constraints the values that the bath energy $E$ can take given a system energy $\varepsilon_{i}$.

### 3.6 Reduced system dynamics: a hierarchy of master equations

In conventional open quantum systems' theory, one is only interested in the evolution of the reduced state of the system $\rho_{\mathrm{S}}$. This state encodes all information that can be extracted by measuring locally the open quantum system at a single time; that is, without considering multi-time statistics [MM21].

With the tools at hand, the reduced dynamics of the system can be obtained in two ways. On the one hand, following Sec. 2.2.3 one can derive the BMS master equation, which is already an equation for the reduced state $\rho_{\mathrm{s}}$. On the other hand, one can derive the EMME and marginalize over the bath energy $E$ to obtain an equation for $\rho_{\mathrm{S}}$. We refer to the resulting equation as the "reduced EMME". While similar in form, the two aforementioned strategies give rise to two different master equations for the reduced state of the system. In this section, we investigate under which circumstances both equations become equivalent.

To remain focused, we assume $\left\langle e_{k}\right| B\left|e_{k}\right\rangle=0$ for all $k$. Also, we assume the system-bath composite to be initialized in the state $\rho(0)=\rho_{\mathrm{S}}(0) \otimes \pi_{\mathrm{B}}^{\prime}\left(\beta_{0}\right)$. We note the prime in the Gibbs state $\pi_{\mathrm{B}}^{\prime}\left(\beta_{0}\right)$, which denotes that the Gibbs state is constructed as

$$
\begin{equation*}
\pi_{\mathrm{B}}^{\prime}\left(\beta_{0}\right)=\int d E \frac{v(E) e^{-\beta_{0} E}}{Z_{\mathrm{B}}^{\prime}\left(\beta_{0}\right)} \omega_{\mathrm{B}}(E) \approx \frac{\exp \left(-\beta_{0} H_{\mathrm{B}}\right)}{\operatorname{tr}\left[\exp \left(-\beta_{0} H_{\mathrm{B}}\right)\right]}=\pi_{\mathrm{B}}\left(\beta_{0}\right), \tag{3.87}
\end{equation*}
$$

where $Z_{\mathrm{B}}^{\prime}(\beta)=\int d E v(E) \exp (-\beta E)$. How well $\pi_{\mathrm{B}}^{\prime}\left(\beta_{0}\right)$ approximates the Gibbs state $\pi_{\mathrm{B}}\left(\beta_{0}\right)$ depends on the choice of the parameter $\delta E$.

For later comparison, we show here the BMS master equation (2.58) in the case of the corresponding Gibbs state $\pi_{\mathrm{B}}^{\prime}\left(\beta_{0}\right)$ for the environment. It yields

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}= & -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}\right]-i\left[H_{\mathrm{S}}^{\mathrm{LS}}\left(\beta_{0}\right), \rho_{\mathrm{S}}\right]+\sum_{\omega} \gamma^{\prime}\left(\beta_{0} ; \omega\right)\left(S_{\omega} \rho_{\mathrm{S}} S_{\omega}^{\dagger}-\frac{1}{2}\left\{S_{\omega}^{\dagger} S_{\omega}, \rho_{\mathrm{S}}\right\}\right) \\
& =: \mathcal{L}_{\mathrm{S}}\left(\beta_{0}\right) \tag{3.88}
\end{align*}
$$

The quantities $H_{\mathrm{S}}^{\mathrm{LS}}\left(\beta_{0}\right)$ and $\gamma^{\prime}\left(\beta_{0} ; \omega\right)$ are defined with respect to the modified Gibbs state $\pi_{\mathrm{B}}^{\prime}\left(\beta_{0}\right)$. More precisely, defining the thermal average of an arbitrary function $f(E)$ as

$$
\begin{equation*}
\langle\langle f(E)\rangle\rangle_{\beta}=\int d E \frac{v(E) \exp (-\beta E)}{Z_{\mathrm{B}}^{\prime}(\beta)} f(E), \tag{3.89}
\end{equation*}
$$

we have that

$$
\begin{align*}
H_{\mathrm{S}}^{\mathrm{LS} \prime}\left(\beta_{0}\right) & =\left\langle\left\langle H_{\mathrm{S}}^{\mathrm{LS}}(E)\right\rangle\right\rangle_{\beta_{0}} \approx H_{\mathrm{S}}^{\mathrm{LS}}\left(\beta_{0}\right),  \tag{3.90}\\
\gamma^{\prime}\left(\beta_{0} ; \omega\right) & =\langle\langle\gamma(E ; \omega)\rangle\rangle_{\beta_{0}} \approx \gamma\left(\beta_{0} ; \omega\right) . \tag{3.91}
\end{align*}
$$

In the following, we assume that $\delta E$ is such that the above approximations are accurate and, consequently, we drop the prime from the notation.

### 3.6.1 The reduced EMME

As we have seen, the central object governing the decoherence of an open quantum system in the weak-coupling regime is the bath correlation function. We have encountered two types of bath correlation functions: the "equilibrium" bath correlation functions $C(\mathbf{a} ; \tau)$, and the "extended" bath correlation functions $C_{m}\left(E, E^{\prime} ; \tau\right)$ that appear in the EMME (3.33). Clearly, there the two types are not fully independent. For instance, given the microcanonical equilibrium correlation function $C(E ; \tau)=\left\langle\delta B(\tau)^{\dagger} \delta B\right\rangle_{E}$, we find the relation

$$
\begin{equation*}
\int d E^{\prime} C_{1}\left(E^{\prime}, E ; \tau\right)=\int d E^{\prime} C_{2}\left(E^{\prime}, E ; \tau\right)=\operatorname{tr}\left[\delta B(\tau)^{\dagger} \delta B \omega_{\mathrm{B}}(E)\right]=C(E ; \tau) . \tag{3.92}
\end{equation*}
$$

We now integrate Eq. (3.33) over the energy $E$ and use the property (3.92) to arrive at the equation

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}}= & -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}\right]-i \int d E\left[H_{\mathrm{S}}^{\mathrm{LS}}(E), \rho_{\mathrm{S}}(E)\right] \\
& +\sum_{\omega} \int d E \gamma(E ; \omega)\left(S_{\omega} \rho_{\mathrm{S}}(E) S_{\omega}^{\dagger}-\frac{1}{2}\left\{S_{\omega}^{\dagger} S_{\omega}, \rho_{\mathrm{S}}(E)\right\}\right) . \tag{3.93}
\end{align*}
$$

where the quantities

$$
\begin{align*}
& H_{\mathrm{S}}^{\mathrm{LS}}(E)=\int d E^{\prime} H_{\mathrm{S}}^{\mathrm{LS}}\left(E^{\prime}, E\right),  \tag{3.94}\\
& \gamma(E ; \omega)=\int d E^{\prime} \gamma_{1}\left(E^{\prime}, E ; \omega\right)=\int d E^{\prime} \gamma_{2}\left(E^{\prime}, E ; \omega\right), \tag{3.95}
\end{align*}
$$

correspond to the definitions given in Sec. 2.2 for the microcanonical state $\omega_{\mathrm{B}}(E)$.
Equation (3.93) is formally similar, but not equivalent, to the BMS master equation (3.88). Clearly, both equations cannot be identical since the EMME can give improved dynamical predictions for certain models, as we have seen in Sec. 3.4. A closer look reveals that Eq. (3.93) is not a closed equation for the reduced state $\rho_{\mathrm{s}}$, since it still depends on the extended states $\rho_{\mathrm{s}}(E)$. Hence, for the prediction of the EMME to coincide with that of the BMS, on needs that the dependence of the reduced EMME on the extended states $\rho_{\mathrm{S}}(E)$ disappears. Below, we discuss under which circumstances this can happen.

### 3.6.2 Two limiting cases

We study here two limiting cases from which the BMS master equation arises from the EMME. The first case (i) corresponds to the situation when the state $\rho_{\mathrm{S}}(E)$ remains approximately uncorrelated at all times; that is, $\rho_{\mathrm{S}}(E) \approx \rho_{\mathrm{S}} p(E)$. Then, one recovers a closed equation for the reduced state of the system in the form

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=-i\left[H_{\mathrm{S}}+\left\langle\left\langle H_{\mathrm{S}}^{\mathrm{LS}}(E)\right\rangle\right\rangle_{p}, \rho_{\mathrm{S}}\right]+\sum_{\omega}\langle\langle\gamma(E ; \omega)\rangle\rangle_{p}\left(S_{\omega} \rho_{\mathrm{S}} S_{\omega}^{\dagger}-\frac{1}{2}\left\{S_{\omega}^{\dagger} S_{\omega}, \rho_{\mathrm{S}}\right\}\right) . \tag{3.96}
\end{equation*}
$$

where $\langle\langle f(E)\rangle\rangle_{p}=\int d E f(E) p(E)$. If, moreover, the distribution $p(E)$ happens to be well approximated by an equilibrium distribution $p(\beta ; E)=Z_{\mathrm{B}}^{-1}(\beta) v(E) \exp (-\beta E)$, then one can replace $\langle\langle\circ\rangle\rangle_{p} \approx\langle\langle\circ\rangle\rangle_{\beta}$ and one recovers exactly Eq. (3.88). However, this limit is unsatisfactory, since dissipation and noise are often a consequence of building and destroying system-bath correlations. More importantly, the limit itself depends on the trajectory of the system-bath evolution rather than on the physical properties of the bath.

There exists a second limit (ii) that causes Eq. (3.93) to reduce to Eq. (3.88). Let $\Delta E$ be the uncertainty associated with the distribution $p(E)$ around the average energy $\mathrm{U}_{\mathrm{B}}=\langle\langle E\rangle\rangle_{p}$. Then, if the $H_{S}^{\mathrm{LS}}(E)$ and $\gamma(E ; \omega)$ are constant over the range of energies $\Delta E$, one can marginalize the state $\rho_{\mathrm{S}}(E)$ over the energy $E$ in Eq. (3.93) to find a closed equation for $\rho_{\mathrm{S}}$ that is formally equal to the BMS. If, moreover, the


Figure 3.4: Sketch of the hierarchy and validity range of the different discussed master equations.
equivalence of ensembles holds for the bath, in the sense that $C\left(\mathrm{U}_{\mathrm{B}}, \tau\right) \approx C(\beta, \tau)$ for the inverse temperature $\beta$, one recovers exactly Eq. (3.88). A similar discussion is conducted in Ref. [EG07].

In the following, we derive a hierarchy of master equations for the reduced state of the system $\rho_{\mathrm{S}}$, which is intuitively summarized as follows. First, the most general master equation that takes into account all the environmental dynamical information is equivalent to unitary evolution and corresponds to the NakajimaZwanzig master equation. Second, an open quantum system that exchanges energy with a weakly coupled finite bath can be described using the EMME, which keeps track of the dynamically evolving bath energy distribution $p(E)$. Third, in some cases it may suffice to keep track of the bath average energy, which is in one-toone correspondence with a certain nonequilibrium effective temperature $\beta^{*}$ (to be defined below). Then, the dynamics is generated by the BMS master equation at this inverse temperature $\beta^{\star}$. Finally, if one fully ignores the finiteness of the bath and assumes it is found in a constant thermal state at inverse temperature $\beta_{0}$, the dynamics are generated by the BMS master equation at this constant temperature. We sketch this hierarchy in Fig. 3.4.

### 3.6.3 A hierarchy of master equations

Finally, we discuss how the promised hierarchy of master equations arises. The philosophy behind the present approach is as follows. Incorporating dynamical information about the environment leads to more accurate predictions about the open system dynamics. In this spirit, we wonder whether it exists a hierarchy of such master equations, where neglecting certain dynamical information about the environment gives rise to simpler master equations, but with a more restricted
range of validity. The answer is positive, and it requires interpolating between the discussed limiting cases (i) and (ii).

Typically, one wants to describe the evolution of a system under conditions that correspond to neither (i) nor (ii), but that can be relatively close to both limits at the same time. To discuss this situation, it is convenient to introduce a perturbative parameter $\eta$ that keeps track of the degree of closeness to (i) and (ii). Namely, we introduce the differences $\delta \rho_{\mathrm{S}}(E):=\rho_{\mathrm{s}}(E)-\rho_{\mathrm{S}} p(E), \delta H_{\mathrm{S}}^{\mathrm{LS}}(E):=H_{\mathrm{S}}^{\mathrm{LS}}(E)-H_{\mathrm{S}}^{\mathrm{LS}}(\beta)$, and $\delta \gamma(E ; \omega):=\gamma(E ; \omega)-\gamma(\beta ; \omega)$, and assume that they are of the same order $\eta$. We now allow the parameter $\beta=\beta(t)$ to depend on time with the initial condition $\beta(0)=\beta_{0}$. Reexpressing Eq. (3.93) in terms of the differences and using that $\int d E \delta \rho_{\mathrm{S}}(E)=0$, we obtain to first order in $\eta$

$$
\begin{align*}
\partial_{t} \rho_{\mathrm{S}} \approx & \approx \mathcal{L}_{\mathrm{S}}(\beta)\left[\rho_{\mathrm{S}}\right]-i\left[\left\langle\left\langle\delta H_{\mathrm{S}}^{\mathrm{LS}}(E)\right\rangle\right\rangle_{p}, \rho_{\mathrm{S}}\right]  \tag{3.97}\\
& +\sum_{\omega}\langle\langle\delta \gamma(E ; \omega)\rangle\rangle_{p}\left(S_{\omega} \rho_{\mathrm{S}} S_{\omega}^{\dagger}-\frac{1}{2}\left\{S_{\omega}^{\dagger} S_{\omega}, \rho_{\mathrm{S}}\right\}\right) .
\end{align*}
$$

Hence, the EMME and the BMS coincide to zeroth order in $\eta$.
Intriguingly, the EMME and the BMS can coincide to first order in $\eta$ provided that we can find a time-dependent inverse temperature $\beta$ such that $\left\langle\left\langle\delta H_{\mathrm{LS}}(E)\right\rangle_{p}\right.$ and $\langle\langle\delta \gamma(E ; \omega)\rangle\rangle_{p}$ vanish for all times. To proceed, we Taylor expand in the energy $E$ around the mean value $\mathrm{U}_{\mathrm{B}}$ to find $H_{\mathrm{LS}}(E) \approx H_{\mathrm{LS}}\left(\mathrm{U}_{\mathrm{B}}\right)+\left[\partial_{E} H_{\mathrm{LS}}(E)\right]_{E=U_{\mathrm{B}}}\left(E-\mathrm{U}_{\mathrm{B}}\right)$ and $\gamma(E ; \omega)=\gamma\left(\mathrm{U}_{\mathrm{B}} ; \omega\right)+\left[\partial_{E} \gamma(E ; \omega)\right]_{E=U_{B}}\left(E-\mathrm{U}_{B}\right)$, which can be done for a sufficiently small $\Delta E$ and a sufficiently smooth bath spectrum. In that case, there always exists a time-dependent choice $\beta(t)$ for which the first order of Eq. (3.97) vanishes. This choice corresponds to the solution $\beta^{\star}$ of the equation

$$
\begin{equation*}
\langle\langle E\rangle\rangle_{\beta^{*}(t)}!=\mathrm{U}_{\mathrm{B}}, \tag{3.98}
\end{equation*}
$$

that is, the inverse temperature of a thermal state that has the same average energy as the actual state of the bath. Therefore, the role of the time-dependent solution of Eq. (3.98) is to update the temperature of the bath according to the current average bath energy. This relation can be made even more apparent by taking the derivative of Eq. (3.98), which leads to

$$
\begin{equation*}
\dot{\beta}^{\star}(t)=-\frac{1}{\mathcal{C}\left(\beta^{\star}(t)\right)} \dot{\mathrm{Q}}(t) \tag{3.99}
\end{equation*}
$$

where $\mathcal{C}(\beta):=d \mathrm{U}_{B} / d \beta$ is the canonical heat capacity with respect to the inverse temperature, and $\dot{\mathrm{Q}}=-\partial_{t} \mathrm{U}_{\mathrm{B}}$ the heat flux. Equation (3.99) explicitly shows that in order to use the BMS master equations for a finite bath, one has to update the bath


Figure 3.5: Sketch of the piecewise non-interacting spin bath. The central system (in blue, label S ) is weakly coupled to several regions (in red, labels $R_{1}, R_{2}, R_{3}, \cdots$ ) that conform a lattice $\mathfrak{L}$.
temperature due to the heat flux exchanged with the system. Only in the limit of an infinite bath, for which the extensive heat capacity $\mathcal{C}\left(\beta^{\star}\right)$ tends to infinity, one is allowed to set $\beta^{\star}(t)=\beta_{0}$ and be still correct to first order in $\eta$ at all times.

Interestingly, the same effective nonequilibrium temperature $\beta^{\star}$ has been proposed as a definition of nonequilibrium temperature in phenomenological nonequilibrium thermodynamics, see Refs. [MB77; Mus77]. Moreover, it has been recently shown to appear in a microscopic derivation of Clausius' inequality [RSS21b; SDR21a; SW21].

### 3.7 Piece-wise non-interacting bath

Having found the hierarchy of master equations, we take now a step back and focus on applying the EMME to study the dynamics of open quantum systems that are in contact with finite baths. From a practical point of view, using Eq. (3.33) to describe the dynamics of an open quantum system requires to compute the extended bath correlation functions $C_{m}\left(E, E^{\prime} ; \tau\right)$ and its half-Fourier transform. This task is setup dependent, and it can be difficult to get an intuition for an arbitrarily general coupling operator $B$ or bath Hamiltonian $H_{B}$. However, there is a relatively
large class of environments for which one can take advantage of arguments of statistical mechanics to proceed further in the calculations. This class corresponds to environments of non-interacting parts that couple locally to the system, which we make precise in the following.

We consider the bath to be embedded in a finite lattice $\mathfrak{L}$. To each lattice site $r \in \mathfrak{L}$ we associate a local Hilbert space of dimension $d(r)$. Then, we partition $\mathfrak{L}=\cup_{R} R$ into regions $R$, and associate to each region $R$ a local Hamiltonian $H_{R}$ that only involves sites $r \in R$ and has dimension $d(R)=\prod_{r \in R} d(r)$. Then, the bath Hamiltonian

$$
\begin{equation*}
H_{\mathrm{B}}=\sum_{R} H_{R}, \tag{3.100}
\end{equation*}
$$

is piecewise non-interacting; i.e., $\left[H_{R}, H_{R^{\prime}}\right]=0$. Importantly, the notion of local is not restricted to spatially local. The structure in Eq. (3.100) could also be, for instance, with respect to momentum space. We sketch this scenario in Fig. 3.5.

We introduce the notation $|n(R)\rangle$ for the $n^{\text {th }}$ excited state of the Hamiltonian $H_{R}$; that is, $H_{R}|n(R)\rangle=e_{n(R)}|n(R)\rangle$. Then, the eigenenergies of the bath Hamiltonian are given by $e_{\mathbf{n}}:=\sum_{R} e_{n(R)}$ where $\mathbf{n}$ is a vector of components $n(R)$. Moreover, we assume that the open quantum system interacts locally with each local $H_{R}$ giving rise to an interaction of the form

$$
\begin{equation*}
H_{\mathrm{int}}=\lambda S \otimes \sum_{R} B_{R} \tag{3.101}
\end{equation*}
$$

where again $B_{R}$ only involves sites $r \in R$. Despite being restrictive, many wellknown models of open quantum systems like the central spin [Gau76] or the Caldeira-Leggett [CL83] model fall in this category.

### 3.7.1 Local correlation functions

With a Hamiltonian of the form (3.100) and an interaction of the form (3.101), the computation of the correlation functions simplifies and can be written as a sum of local correlation functions; for instance, $\langle\tilde{B}(\tau) B\rangle_{E^{\prime}}=\sum_{R}\left\langle B_{R}(\tau) B_{R}\right\rangle_{E^{\prime}}$. We start considering the computation of the correlation function

$$
\begin{equation*}
\left\langle B_{R}(\tau) B_{R}\right\rangle_{E^{\prime}}=\operatorname{tr}_{R}\left\{B_{R}(\tau) B_{R} \operatorname{tr}_{\bar{R}}\left[\omega_{\mathrm{B}}\left(E^{\prime}\right)\right]\right\}, \tag{3.102}
\end{equation*}
$$

where $\bar{R}$ is the complementary set of $R$; that is, $R \cup \bar{R}=\mathfrak{L}$. The trace over $\bar{R}$ can be now performed as follows. Define the conditional POVM elements

$$
\begin{align*}
P(E \mid n(R)): & :=|n(R) \times n(R)| P(E)|n(R) \times n(R)| \\
& =\sum_{\overline{\mathbf{n}}} W\left(E \mid e_{n(R)}+e_{\mathbf{n}}\right)|n(R), \overline{\mathbf{n}} \times n(R), \overline{\mathbf{n}}|, \tag{3.103}
\end{align*}
$$

where $\overline{\mathbf{n}}$ sums over the complementary components of $n(R)$ and also define the corresponding conditional volumes $v(E \mid n(R))=\operatorname{tr}[P(E \mid n(R))]$. Then, we arrive at the exact formula

$$
\begin{equation*}
\Phi_{R}(E)=\operatorname{tr}_{\bar{R}}\left[\omega_{\mathrm{B}}(E)\right]=\sum_{n(R)} \frac{v(E \mid n(R))}{v(E)}|n(R) \times n(R)|, \tag{3.104}
\end{equation*}
$$

for the reduced state of the subsystem $R$. With the help of the reduced states $\Phi_{R}(E)$, we can simply compute the correlation function as a sum of local terms as

$$
\begin{equation*}
C(E ; \tau)=\sum_{R} \operatorname{tr}_{R}\left[B_{R}(\tau) B_{R} \Phi_{R}(E)\right] . \tag{3.105}
\end{equation*}
$$

### 3.7.2 Emergent Gibbs distribution

Despite being formally exact, the expression of the correlation function $C(E ; \tau)$ is not yet transparent. In particular, we would like to attach a physical meaning to the ratio of volume terms appearing in the reduced state $\Phi_{R}(E)$. To this end, we use a well-known argument from statistical mechanics. While we expect this argument to work for typical baths, we have to make further assumptions to derive it formally.

Namely, we assume that $(i)$ the weighting functions to be only a function of the difference $W\left(E \mid e_{k}\right)=W\left(E-e_{k}\right)$; (ii) the volumes fulfill $v(E \mid n(R)) \approx d(R) v\left(E-e_{n(R)}\right)$; and (iii) the Boltzmann-Planck entropy $\mathrm{S}_{\mathrm{BP}}(E)=\log [v(E) \delta E]$ is a sufficiently slowly varying function of $E$ and can be Taylor expanded to first order at the local energy scale $e_{n}(R)$.

Assumption ( $i$ ) is to be expected in many practical cases. For instance, both $W_{\mathrm{I}}\left(E \mid e_{k}\right)$ and $W_{\mathrm{G}}\left(E \mid e_{k}\right)$ fall in this category. Assumption (ii), is expected for large baths where the eigenstate distribution of $\bar{R}$ has reached its limiting value, and attaching to it the extra region $R$ is equivalent to multiplying the limiting distribution by the local dimension $d(R)$. Finally, assupmtion (iii) is also to be expected for large baths with many regions $R$, since the local energies $e_{n}(R)$ are a small contribution to the total energy. Then, with the help of the Boltzmann inverse temperature $\beta(E):=\frac{\partial}{\partial E} \mathrm{~S}_{\mathrm{BP}}(E)$ one can expand $\mathrm{S}_{\mathrm{BP}}\left(E-e_{n(R)}\right) \approx \mathrm{S}_{\mathrm{BP}}(E)-\beta(E) e_{n(R)}$.

Putting assumptions (i)-(iii) together, we arrive at the well-known result of statistical mechanics that the Gibbs distribution arises as measuring locally a system in a global microcanonical state at a given energy E [LL13]. In our notation,

$$
\begin{equation*}
\Phi_{R}(E)=\operatorname{tr}_{\bar{R}}\left[\omega_{\mathrm{B}}(E)\right] \approx \sum_{n(R)} \frac{e^{-\beta(E) e_{n(R)}}}{Z_{\mathrm{R}}(\beta(E))}|n(R) \times n(R)|=\pi_{R}\left(\beta_{\mathrm{B}}(E)\right), \tag{3.106}
\end{equation*}
$$

where $Z_{R}(\beta)=\sum_{n(R)} \exp \left(-\beta e_{n(R)}\right)$. Finally, we believe that the above assumptions are not crucial to the derivation of Eq. (3.106), since the thermal state has been shown to arise as the correct reduced state for the overwhelming majority of quantum states [GLT+06; PSW06].

### 3.7.3 Kubo-Martin-Schwinger relation

Interestingly, exploiting the emergent thermal distribution discussed of the last subsection, one recovers the Kubo-Martin-Schwinger relation that governs the equilibrium properties under the BMS master equation as we saw in Sec. 2.5.3. In particular, we note that the correlation function fulfill

$$
\begin{equation*}
C(E ; \tau) \approx \sum_{R} \operatorname{tr}_{R}\left[B_{R}(\tau) B_{R} \pi_{R}\left(\beta_{\mathrm{B}}(E)\right)\right]=: \sum_{R} C_{R}\left(\beta_{\mathrm{B}}(E) ; \tau\right) . \tag{3.107}
\end{equation*}
$$

where $C_{R}(\beta ; \tau)$ are thermal correlation functions for the region $R$. Because each region has a thermal correlation function, we see that

$$
\begin{equation*}
C(E ; \tau)=\sum_{R} C_{R}\left(\beta_{\mathrm{B}}(E) ;-\tau-i \beta_{\mathrm{B}}(E)\right)=C\left(E ;-\tau-i \beta_{\mathrm{B}}(E)\right) . \tag{3.108}
\end{equation*}
$$

Therefore, we find that the dissipation rates obey

$$
\begin{equation*}
\gamma(E ;-\omega)=\lambda^{2} \int_{\mathbb{R}} d \tau C\left(\beta ;-\tau-i \beta_{\mathrm{B}}(E)\right) e^{-i \omega \tau}=e^{-\beta(E) \omega} \gamma(E ; \omega) . \tag{3.109}
\end{equation*}
$$

Crucially, because the Boltzmann temperature depends on the energy this does not always lead to a Gibbs state for the system as the stationary distribution.

### 3.8 Example: Central spin model

In this section, we use the EMME to numerically investigate the dynamics of a spin system coupled to a bath of non-interacting spin- $1 / 2$ particles, which is also known as the central spin model (see Fig. 3.6 for a sketch). This bath for this model is a piecewise non-interacting bath, which allows us to take advantage of the results of Sec. 3.7. Central spin baths describe the effect of an environment dominated by localized modes, such as nuclear spins, paramagnetic spins, or defects [PS00]. Hence, they are suitable to describe the interaction of a spin system embedded in an environment which contains many other spin degrees of freedom; such as nitrogenvacancy centers in diamond [LSC+13; SLC+14; SST+18] or quantum dots [HKP+07; UMA+13].


Figure 3.6: Sketch of the central spin model, where the central spin has an energy scale $\omega_{\mathrm{S}}$ and the spins in the bath have different energy splittings $\Omega_{r}$. The interaction strength between the system and the spins in the environment is of order $\lambda$.

Ultimately, the aim of this section is to investigate the hierarchy of master equations that we have discussed in Sec. 3.6.3 for the central spin model. To this end, we start computing the volume terms $v(E)$ and correlation functions $C_{m}\left(E, E^{\prime} ; \omega\right)$ for the central spin model and afterwards finding the corresponding EMME.

### 3.8.1 The spin bath: volumes and correlation functions

We start studying the properties of the spin bath, which consists of a collection of $N_{s}$ spin- $1 / 2$ particles, which are microscopically described by the Hamiltonian

$$
\begin{equation*}
H_{\mathrm{B}}=\sum_{r=1}^{N_{s}} \frac{\Omega_{r}}{2} \sigma_{r}^{z}, \tag{3.110}
\end{equation*}
$$

where $\sigma_{r}^{x, y, z}$ and $\Omega_{r}$ are respectively the Pauli matrices and the Zeeman energy of the $r^{\text {th }}$ spin. Its eigenenergies are given by

$$
\begin{equation*}
e_{\mathbf{n}}:=\sum_{r=1}^{N_{s}} n_{r} \frac{\Omega_{r}}{2} \tag{3.111}
\end{equation*}
$$

where $\mathbf{n}=\left(n_{1}, \cdots, n_{N_{s}}\right)$ has components $n_{r} \in\{-1,1\}$. We consider that the frequencies $\Omega_{r}$ to be sampled from a given underlying probability distribution $\varrho(\Omega)$ with average $\Omega_{0}$ and variance $\sigma_{\Omega}$.

Interestingly, every energy $e_{\mathrm{n}}$ can be regarded as the endpoint of a random walk of $N_{s}$ steps and random step sizes $\Omega_{r} / 2$. In that scenario, the central limit
theorem applies (see App. B.3) and the distribution of end points is given by a normal distribution of variance $\sigma_{N_{s}}^{2}$

$$
\begin{equation*}
\sigma_{N}^{2}=\sum_{r=1}^{N_{s}} \frac{1}{2}\left[\left(\frac{\Omega_{r}}{2}\right)^{2}+\left(-\frac{\Omega_{r}}{2}\right)^{2}\right]=\sum_{r=1}^{N_{s}} \frac{\Omega_{r}^{2}}{4} \tag{3.112}
\end{equation*}
$$

Then, it is then possible to approximate the density of states of the bath

$$
\begin{equation*}
g(e):=\sum_{\mathbf{n}} \delta\left(e-e_{\mathbf{n}}\right) \approx \frac{2^{N_{s}}}{\sqrt{2 \pi} \sigma_{N_{s}}} \exp \left(-\frac{e^{2}}{2 \sigma_{N_{s}}^{2}}\right) . \tag{3.113}
\end{equation*}
$$

In the top-left panel of Fig. 3.7, we compare the histogram of the exact spectrum with the normalized Gaussian fit in Eq. (3.113), showing a very good agreement.

With the density of states at hand, we can proceed to compute the volume terms $v(E)$. In terms of the density of states $g(e)$, the volumes can be written as

$$
\begin{equation*}
v(E)=\int \operatorname{deW}(E \mid e) g(e) . \tag{3.114}
\end{equation*}
$$

We can find closed expressions for the volume terms in the cases of $W_{\mathrm{I}}\left(E \mid e_{k}\right)$ and $W_{\mathrm{G}}\left(E \mid e_{k}\right)$. They read respectively

$$
\begin{align*}
& v_{\mathrm{I}}\left(E_{x}\right) \approx \frac{2^{N_{s}-1}}{\delta E}\left[\operatorname{erf}\left(\frac{E_{x}+\delta E / 2}{\sqrt{2} \sigma_{N_{s}}}\right)-\operatorname{erf}\left(\frac{E_{x}-\delta E / 2}{\sqrt{2} \sigma_{N_{s}}}\right)\right] \\
& v_{\mathrm{G}}(E) \approx \frac{2^{N_{s}}}{\sqrt{2 \pi\left(\delta E^{2}+\sigma_{N_{s}}^{2}\right)}} \exp \left[-\frac{E^{2}}{2\left(\delta E^{2}+\sigma_{N_{s}}^{2}\right)}\right] \tag{3.115}
\end{align*}
$$

where $\operatorname{erf}(x)$ is the error function, and which become equivalent in the limit $\delta E \rightarrow 0$.
Provided the analytical expressions for the volumes $v_{\mathrm{I}}(E)$ and $v_{\mathrm{G}}(E)$, we can also compute analytically the Boltzmann-Planck entropy $\mathrm{S}_{\mathrm{BP}}(E)$ taking the logarithm. In particular, for the Gaussian volume $v_{\mathrm{G}}(E)$, we find the linear relation $\beta_{\mathrm{B}}(E)=-E / \sigma_{N_{s}}^{2}$, between the Boltzmann temperature and the energy $E$. The same relation also holds for $v_{\mathrm{I}}\left(E_{x}\right)$, provided that $\delta E /\left(\sqrt{2} \sigma_{N_{s}}\right)$ is small enough to Taylor expand the error function $\operatorname{erf}(x+\delta x) \approx \operatorname{erf}(x)+\exp \left(x^{2}\right) \delta x / \sqrt{\pi}$. Interestingly, the microcanonical heat capacity for this model turns out to be a constant $C(\beta(E))=-\sigma_{N_{s}}^{2}$ which, as expected, is extensive with the number of spins $N_{s}$.

The next step is computing the bath correlation functions $C\left(E, E^{\prime} ; \tau\right)$ for the central spin model. To this end, we need to specify the interaction Hamiltonian which we take to be

$$
\begin{equation*}
H_{\mathrm{int}}=\lambda S \otimes \sum_{r=1}^{N_{s}} c_{r} \sigma_{r}^{x} \tag{3.116}
\end{equation*}
$$



Figure 3.7: (top-left) Histogram of eigenstates for the central spin bath and comparison with the approximate normalized density of states (solid orange line) for $N_{s}=14$ spins; (top-right) Ratio of the computation of $f\left(E_{x}, E_{x^{\prime}} ; \Omega\right)$ using the exact Eq. (3.118) over the approximated Eq. (3.119) expressions as a function of the number of spins $N_{s}$, with $E_{x}=-2 \delta E, E_{x^{\prime}}=-\delta E$, and $\Omega=\delta E$; (bottom-left) Real (solid orange line) and imaginary (dashed blue line) parts of the correlation function $C\left(E_{x}, E_{x^{\prime}} ; \tau\right)$ as a function of time for $N_{s}=300$ spins, with $E_{x}=-8 \delta E$ and $E_{x^{\prime}}=-9 \delta E$; (bottom-right) Comparison of the analytical approximation (solid orange line) and the numerical calculation (blue dashed line) corresponding to the correlation function of the bottom-left panel with $\lambda=0.01 \delta E$. In all panels, the frequencies $\Omega_{r}$ are distributed according to a normal distribution of mean $\Omega_{0}=\delta E$ and variance $\sigma_{\Omega}=0.2 \delta E$.

We note that $H_{\mathrm{B}}$ and $H_{\text {int }}$ have the form given by (3.100) and (3.101) respectively. In particular, the regions $R$ contain a single site $r$ and the corresponding Hamiltonians $H_{r}=\Omega_{r} \sigma_{r}^{z} / 2$ have dimension $d(R)=d(r)=2$. Therefore, the correlation function can be computed as a sum of local terms, and we find

$$
\begin{equation*}
C_{1}\left(E, E^{\prime} ; \tau\right)=\frac{1}{v\left(E^{\prime}\right)} \sum_{r=1}^{N_{s}} c_{r}^{2}\left[e^{-i \Omega_{r} \tau} f\left(E, E^{\prime} ; \Omega_{r}\right)+e^{i \Omega_{r} t} f\left(E, E^{\prime} ;-\Omega_{r}\right)\right] . \tag{3.117}
\end{equation*}
$$

In Eq. (3.117) we have introduced the function

$$
\begin{equation*}
f\left(E, E^{\prime} ; \Omega_{r}\right)=\sum_{\overline{\mathbf{n}}} W\left(E \mid e_{\overline{\mathbf{n}}^{\prime}}+\Omega_{r} / 2\right) W\left(E^{\prime} \mid e_{\overline{\mathbf{n}}}-\Omega_{r} / 2\right), \tag{3.118}
\end{equation*}
$$

that has the symmetry $f\left(E, E^{\prime} ; \Omega_{r}\right)=f\left(E^{\prime}, E ;-\Omega_{r}\right)$. An exact computation of $f\left(E, E^{\prime} ; \Omega_{r}\right)$ is in general only available through numerical calculation. However, we can make use of the density of states $g(e)$ in Eq. (3.113) to approximate

$$
\begin{equation*}
f\left(E, E^{\prime} ; \Omega_{r}\right) \approx \frac{1}{2} \int \operatorname{deg}(e) W\left(E \mid e+\Omega_{r} / 2\right) W\left(E^{\prime} \mid e-\Omega_{r} / 2\right) . \tag{3.119}
\end{equation*}
$$

where we have used that, for a sufficiently large $N_{s}$, removing a particle approximately scales down $g(e)$ by a factor of two. In the top-right panel of Fig. 3.7, we show the ratio of the exact value of $f\left(E, E^{\prime} ; \Omega\right)$ in Eq. (3.118) over its approximated value as computed with Eq. (3.119) as a function of the number of spins $N_{s}$. One observes that, for a sufficiently large number of particles $N_{s} \sim 12$, it is justified to use Eq. (3.119) to evaluate the function $f\left(E, E^{\prime} ; \Omega_{r}\right)$.

In the derivation of the EMME, we have used that the correlation functions decay rapidly in time. This approximation is crucial to obtain a time-independent equation for the evolution of $\rho_{\mathrm{S}}(E)$ and thus, its validity has to be assessed. With the help of $g(e)$ it is possible to evaluate efficiently the correlation function $C_{m}\left(E, E^{\prime} ; \tau\right)$, for $m=1,2$, for a large number of particles. In the bottom-left panel of Fig. 3.7 we show the $C_{1}\left(E_{x}, E_{x^{\prime}} ; \tau\right)$ as a function of $\tau$ for a particular choice of $E_{x}=-9 \delta E$, $E_{x^{\prime}}=-8 \delta E$ for a bath of $N_{s}=300$ spin- $1 / 2$ particles. We show the decay of the correlation functions as a function of time for a particular choice of the energies $E$ and $E^{\prime}$. As we discussed, the decay of the correlation function is an indicator for the validity of the Markovian approximation.

Ultimately, we are interested in computing the dissipation rates; for instance $\gamma_{1}\left(E, E^{\prime} ; \Omega\right)$, that enter the EMME. If the number of spins of the bath is very large and their splittings $\Omega_{r}$ densely fill a spectral region, the dissipation rates are conveniently written in terms of the spectral density $J(\Omega)=2 \pi \lambda^{2} \sum_{r} c_{r}^{2} \delta\left(\Omega-\Omega_{r}\right)$ defined for $\Omega \geq 0$.

Continuing $J(\Omega)$ towards negative frequencies as $J(-\Omega)=J(\Omega)$ we find the relation

$$
\begin{equation*}
\gamma_{1}\left(E, E^{\prime} ; \Omega\right)=J(\Omega) f\left(E, E^{\prime} ; \Omega\right) / V\left(E^{\prime}\right) . \tag{3.120}
\end{equation*}
$$

We note that, for a spin-independent coupling $c_{r}=1$ for all $r$, the spectral density is linked to the distribution of Zeeman energies through

$$
\begin{equation*}
J(\Omega)=2 \pi \lambda^{2} \sum_{r=1}^{N_{s}} \delta\left(\Omega-\Omega_{r}\right) \approx 2 \pi \lambda^{2} N_{s} \varrho(\Omega) \tag{3.121}
\end{equation*}
$$

where the approximated sign holds exactly in the limit $N_{s} \rightarrow \infty$. In the bottom-right panel of Fig. 3.7, we compare the numerical value of the dissipation rates $\gamma_{1}\left(E, E^{\prime} ; \Omega\right)$ versus its analytic value in Eq. (3.120), where the function $f\left(E, E^{\prime} ; \Omega\right)$ is computed using Eq. (3.119). We find a good agreement between both expressions $N_{s}=300$, which improves increasing $N_{s}$.

### 3.8.2 Comparison between the master equations

Finally, we compare the dynamics generated by the EMME and those generated by the BMS with the effective nonequilibibrium temperature $\beta^{\star}(t)$ and at the constant temperature $\beta_{0}$. At this point, we have to specify the system Hamiltonian $H_{\mathrm{S}}$ and the system interaction $S$. We consider a particle of spin-s with $H_{S}=\omega_{0} S^{z}$ and $S=2 S^{x}$, being $\omega_{S}$ the central spin frequency, and $S^{x}$ and $S^{z}$ are the central spin operators. In the energy eigenbasis the spin operators read

$$
\begin{align*}
& S^{z}=\sum_{i=0}^{2 \mathrm{~s}}(i-\mathrm{s})|i \times i|, \\
& 2 S^{x}=\sum_{i=0}^{2 s-1} \sqrt{(i+1)(2 s-i)}|i \times i+1|+\text { h.c. } \tag{3.122}
\end{align*}
$$

For instance, for a spin- $1 / 2$ particle, we have $H_{S}=\omega_{0} \sigma_{0}^{z} / 2$ and $S=\sigma_{0}^{x}$, being $\sigma_{0}^{z}$ and $\sigma_{0}^{x}$ the standard Pauli operators of the central spin. For simplicity, we consider only the weighting function $W_{\mathrm{I}}\left(E_{x} \mid e_{k}\right)$ where the energies $E_{x}=x \delta E$ with $x \in \mathbb{Z}$; i.e, we coarse-grain the bath energies into non-overlapping energy windows. With this choice of weighting function, we have the relation $\gamma_{2}\left(E_{x}, E_{x^{\prime}} ; \omega\right)=\delta_{x, x^{\prime}} \sum_{x^{\prime \prime}} \gamma_{1}\left(E_{x^{\prime \prime}}, E_{x} ; \omega\right)$.

It is convenient to gather the probabilities $p\left(\varepsilon_{i}, E_{x}\right)$ into the probability vector $\mathbf{p}$ and to define the stochastic matrix $\Lambda$ with off-diagonal elements $\Lambda\left(\varepsilon_{i}, E_{x} ; \varepsilon_{j}, E_{x^{\prime}}\right)=$


Figure 3.8: (left-column) Comparison between the EMME dynamics (solid orange line), the BMS with the effective nonequilibrium temperature $\beta^{\star}(t)$ (blue dashed line), and the BMS at fixed temperature $\beta_{0}$ (yellow dotted line) for: (top-row) the first excited state of a spin- $1 / 2$ particle and (bottom-row) the third excited state of a spin-10 particle; (right-column) corresponding evolution of the effective nonequilibrium temperature (solid orange line). Initially, the system-bath composite is found in the state $\rho(0)=|2 s \times 2 s| \otimes \pi_{\mathrm{B}}\left(\beta_{0}\right)$ with $\beta_{0}=0.75 \delta E$. We take the parameters $N_{s}=100$ spins, $\omega_{0}=\delta E, \lambda=0.01 \delta E, \Omega_{0}=\delta E, \sigma_{\Omega}=0.2 \delta E$, and a spin independent coupling $c_{r} \rightarrow 1$.


Figure 3.9: (left-column) Comparison between the stationary distributions of the system $p^{\text {st }}\left(\varepsilon_{i}\right)$ and the bath $p^{\text {st }}\left(E_{x}\right)$ as predicted for the EMME dynamics (solid oragne line), the BMS with the effective nonequilibrium temperature $\beta^{\star}(t)$ (blue dashed line), and the BMS at fixed temperature $\beta_{0}$ (yellow dotted line) for the same initial states and parameters than Fig. 3.8. (top-row) the first excited state of a spin-1/2 particle and (bottom) the third excited state of a spin-10 particle; (right-column) corresponding evolution of the effective non-equilibrium temperature (solid orange line). Initially, the system-bath composite is found in the state $\rho(0)=|2 s \times 2 s| \otimes \pi_{\mathrm{B}}\left(\beta_{0}\right)$ with $\beta_{0}=0.75 \delta E$. We take the parameters $N_{s}=100 \mathrm{spins}, \omega_{0}=\delta E, \lambda=0.01 \delta E$, $\Omega_{0}=\delta E, \sigma_{\Omega}=0.2 \delta E$, and a spin independent coupling $c_{r} \rightarrow 1$.
$|\langle i| S| j\rangle\left.\right|^{2} \gamma_{1}\left(E_{x}, E_{x^{\prime}} ; \omega_{j i}\right)$, and the diagonal ones determined by the probability conservation condition $\sum_{i, x} \Lambda\left(\varepsilon_{i}, E_{x} ; \varepsilon_{j}, E_{x^{\prime}}\right)=0$. Then, we can compactly write the population evolution equaiton as

$$
\begin{equation*}
\partial_{t} \mathbf{p}=\Lambda \mathbf{p} \tag{3.123}
\end{equation*}
$$

Using the results of Sec. 3.7.1, we explicitly find the off-diagonal elements

$$
\begin{equation*}
\left.\Lambda\left(\varepsilon_{i}, E_{x} ; \varepsilon_{j}, E_{x^{\prime}}\right)=|\langle i| S| j\right\rangle\left.\right|^{2} J\left(\omega_{j i}\right) \frac{f\left(E_{x}, E_{x^{\prime}} ; \omega_{j i}\right)}{v\left(E_{x^{\prime}}\right)} \tag{3.124}
\end{equation*}
$$

with the matrix elements of the system coupling operator

$$
\begin{equation*}
\left.\left|\langle i| 2 S^{x}\right| j\right\rangle\left.\right|^{2}=\delta_{i, j-1}(i+1)(2 s-i)+\delta_{i, j+1} i(2 s-i+1) \tag{3.125}
\end{equation*}
$$

In Fig. 3.8, we show a comparison between the EMME dynamics, the BMS with the effective nonequilibrium temperature $\beta^{\star}(t)$, and the BMS at the fixed inverse temperature $\beta_{0}$ for a particle of (left-column) spin $\mathrm{s}=1 / 2$ and (right-column) $\operatorname{spin} s=10$. For a spin- $1 / 2$ particle, the amount of energy transferred from the system to the bath is very small as compared to the bath average energy. Hence, during the evolution the effective nonequilibrium temperature $\beta^{\star}(t)$, in one to one correspondence with the average energy, remains constant. Hence, the infinite bath approximation is well justified in this situation, and the three master equations coincide. Instead, an initially excited spin- 10 particle is able to transfer a nonnegligible amount of energy to the bath. This is observed in the dynamics of the non-equilibrium temperature $\beta^{\star}(t)$, which changes substantially. As a result, the three master equations give rise to a distinguishable dynamics, as we can see in the bottom-left panel of Fig. 3.8.

Of course, the dependence on the spin, playing the role of the system-size, of these dynamics is reflected in the stationary distributions. In Fig. 3.9, we show the stationary distributions for the system (left-column) and the bath (right-column) for a (top-row) spin-1/2 particle and (bottom-row) spin-10 particle. Similarly to the time-dependent dynamics, the three stationary distributions agree for the system and the bath for the spin- $1 / 2$ particle in the top row. Instead, they become substantially different for a large spin-10 central particle.

### 3.8.3 System-bath correlations

One of the special features of the EMME is that it is capable to describe the evolution of part of the system-bath correlations. Those correlations can be present either


Figure 3.10: (left) System-bath correlations as measured by the classical mutual information for a state of the bath in a microcanonical state $\omega_{\mathrm{B}}\left(E_{x}\right)$ with $E_{x}=-22 \delta E$ and corresponding Boltzmann temperature $\beta(E) \approx 0.83 \delta E^{-1}$ (orange solid and yellow dotted lines); or a canonical state at initial inverse temperature $\beta_{0}=0.75 \delta E^{-1}$ (blue dashed and purple dotdashed lines). The central particle has a spin of $s=1 / 2$ (solid orange and blue dashed lines) or $s=10$ (yellow dotted and purple dotdashed lines). The horizontal gray dashed lines correspond to the maximal value of the mutual information $\log (2 s+1)$ for $s=1 / 2$ and $s=10$. (right) Magnitude of the matrix elements of $\Lambda$ as a function of the position in the basis $\left\{\cdots, p\left(-\omega_{0} / 2, E_{x}+\right.\right.$ $\left.\delta E), p\left(\omega_{0} / 2, E_{x}\right), \cdots\right\}$ for a spin- $1 / 2$ particle. The color white is used to mark elements whose order of magnitude is smaller or equal than $10^{-10}$. The rest of the parameters are set to $N_{s}=100, \omega_{0}=\delta E, \Omega_{0}=\delta E, \sigma_{\Omega}=0.2 \delta E, c_{r}=1$, and $\lambda=0.01 \delta E$.
in the initial system-bath state $\rho(0)$ or can be developed during the system-bath interaction. It is sometimes assumed that, in the weak-coupling limit, system-bath correlations are negligible. Here, we briefly investigate whether this is the case for the central spin model. To this end, we will take advantage of the "classical" mutual information $I_{\mathrm{S}: \mathrm{B}}^{\mathrm{cl}}\left(\left\{p\left(\varepsilon_{i}, E\right)\right\}\right)$ in Eq. (3.85). The mutual information is zero if and only if the system and bath are uncorrelated, and it is upper bounded by $\log d_{s}$, where $d_{\text {S }}$ is the system dimension (assuming the dimensionality of the bath is larger).

In the left panel of Fig. 3.10, we show the evolution of $I_{\mathrm{S}: \mathrm{B}}^{\mathrm{cl}}(\mathbf{p})$ as a function of time. We observe that if the initial state of the bath is canonical $\pi_{\mathrm{B}}(\beta)$, systembath correlations remain small throughout the evolution. However, if the bath starts in a microcanonical state $\omega_{\mathrm{B}}(E)$, system-bath correlations grow close to their maximum possible value. Therefore, system-bath correlations can grow close to their maximum value even in the weak-coupling limit. Physically speaking, the reason why is that the EMME dynamics is constrained by the total energy conservation as we investigated in Sec. 3.5.1. This give rise to a dynamics with many conserved quantities giving rise to an approximate block-structure for the dynamical matrix $\Lambda$ as it can be observed in the right panel of Fig. 3.10. Hence, starting with a microcanonical state leads to stronger system-bath correlations, since the value of the stochastic variable $E_{x}$ is determined by $E_{x}=\mathrm{U}_{\mathrm{B}}-\varepsilon_{i}$.

### 3.9 Chapter's outlook

John von Neumann once said that "truth... is much too complicated to allow anything but approximations". Although controversial, this quotation holds undoubtedly a part of truth. Reality is complicated, practically unsolvable, and, as physicists, we have to find models which capture what is essential and disregard what is not.

In this chapter, we have discussed what a finite bath is and why we expect it to evolve dynamically. Then, starting from the from the fundamental laws of quantum mechanics, we derived an effective master equation that describes the evolution of an open quantum system in contact with a dynamically evolving bath, from which we have access only to coarse-grained properties. To build some intuition, we have introduced a toy model that can be solved exactly (numerically), and we have benchmarked our master equation against the exact dynamics showing very good agreement.

Then, we proceed to investigate the general properties of our master equation. Importantly, we have found that the system plus bath energy is conserved and we have obtained the stationary distribution of our master equation.

The Born-Markov-secular master equation has to arise, in the appropriate limit, from our master equation. Studying how this transition happens, we have found a hierarchy of master equations that give more accurate predictions of the dynamics by including more dynamical bath information. In particular, the middle level of the hierarchy has an associated effective nonequilibrium inverse temperature, which is in one to one correspondence with the bath average energy.

In the following chapter, we explore how this dynamical description can be complemented with a nonequilibrium thermodynamic framework, from which the laws of thermodynamics emerge from the current microscopic description.

## 4

## Nonequilibrium thermodynamics for finite baths

In the previous chapter, we have derived the EMME (3.9) starting from a microscopic description of the system and the bath. One motivation to derive such a master equation is its potential to describe small quantum devices including heat engines, refrigerators or heat pumps. If the bath is finite, operating those small quantum devices can cause the bath to develop nonequilibrium features during the evolution and then, the standard approach relying on a large bath in a Gibbs state cannot be applied. In this respect, it is important to obtain a consistent (nonequilibrium) thermodynamic interpretation of the dynamics.

While the discussion of imperfect measurements was useful in the last chapter, in the present one we remain focused on the case of projective measurements. Hence, we have in mind a coarse-grained description of the bath Hamiltonian $\left\{H_{\mathrm{B}}\right\}:=\sum_{x} E_{x} \Pi\left(E_{x}\right)$, where the energy projectors $\Pi\left(E_{x}\right)=\sum_{k} 1_{E_{x}}\left(e_{k}\right)\left|e_{k} \times e_{k}\right|$ and $E_{x}=x \delta E$, with $x \in \mathbb{Z}$.

This chapter is devoted to study the implications of the master equation approach derived in the Ch. 3 to quantum thermodynamics (or quantum statistical mechanics). In particular, we start discussing how to extend the EMME to include slow driving and multiple heat baths. Then, we define the thermodynamic quantities of interest, like internal energy or entropy, that give rise to the first and second
laws of thermodynamics with our dynamical description. Also, we connect the first and second law with Clausius inequality. While we keep the discussion general, we occasionally illustrate our findings with certain models. In particular, we revisit the Random Matrix bath model studied in Sec. 3.4. Also, we discuss the SWAP engine together with the repeated interaction scheme. The discussion of this chapter is largely based on the two publications [RSS21b] and [SDR21b].

### 4.1 Slow driving and multiple heat baths

The EMME is primarily a tool for describing nonequilibrium physics. In particular, it is able to capture three nonequilibrium sources: (i) A non-thermal initial state $\rho(0)$ of the system and bath composite, (ii) a time-dependent system energy spectrum $\varepsilon_{i}\left(\xi_{t}\right)$, where $\xi_{t}$ represents a sufficiently slow driving protocol ( $\dot{\xi}_{t} \delta t \ll 1$ ), and (iii) the system $S$ being in contact with multiple environments. So far, we have only shown how to explore (i); that is, how to incorporate initial states which are not in the usual form $\rho(0)=\rho_{\mathrm{S}}(0) \otimes \pi_{\mathrm{B}}(\beta)$ but can, in principle, contain system-bath correlations and non-Gibbs bath states.

Those nonequilibrium sources are of interest to the study of quantum thermodynamics. In particular, the time-dependent energies (ii) introduce the notion of work, while multiple heat baths (iii) give rise to local heat currents. Hence, before going into deriving the laws of thermodynamics, it is convenient to extend the EMME to those scenarios.

It is possible to include a slow time-dependent driving of the system energies $\varepsilon_{i}\left(\xi_{t}\right)$ analogously to Sec. 2.6. Namely, if the driving is slow; that is, $\dot{\xi}_{t}$ is small, one is able to substitute directly $\varepsilon_{i} \mapsto \varepsilon_{i}\left(\xi_{t}\right)$ in Eq. (3.9). Intuitively, if at time $t$, given a time step $\delta t$, we can neglect $\xi_{t} \delta t \ll 1$, then one can derive the generator of the EMME with the energies $\varepsilon_{i}\left(\xi_{t}\right)$. Then, at the next time step, one has to repeat the derivation but updating the energies to the value $\varepsilon_{i}\left(\xi_{t+\delta t}\right)$ and iterate.

The third nonequilibrium source (iii) can be also treated analogously to Sec. 2.5.4. Consider multiple baths labeled by the Greek letter $v$, each of them with Hamiltonian $H_{v}$ and coupled to the system with an interaction $H_{\text {int }}=\lambda \sum_{v} S_{v} \otimes B_{v}$. Let $\delta E_{v}$ denote the coarse-graining energy scale with respect to the $v^{\text {th }}$ bath. Then, one can coarsegrain in the usual sense each bath Hamiltonian $H_{v}$ into non-overlapping energy windows to obtain $\left\{H_{v}\right\}=\sum_{x_{v}} E_{x_{v}} \Pi\left(E_{x_{v}}\right)$ with energies $E_{x_{v}}=x_{v} \delta E_{v}$ with $x_{v} \in \mathbb{Z}$. For notational convenience, we introduce the vector $\mathbf{x}=\left(x_{1}, \cdots, x_{v}, \cdots\right)$. Then, the projector $\Pi\left(E_{\mathbf{x}}\right)=\Pi\left(E_{x_{1}}\right) \otimes \cdots \Pi\left(E_{x_{v}}\right) \otimes \cdots$ is the product of the local projectors.

In the case of multiple heat baths, the EMME corresponds to an evolution
equation for $\rho_{\mathrm{S}}\left(E_{\mathbf{x}}\right):=\operatorname{tr}_{\mathrm{B}}\left[\rho \Pi\left(E_{\mathbf{x}}\right)\right]$. This is achieved introducing the relevant map

$$
\begin{equation*}
\mathcal{P}[\circ]=\sum_{\mathbf{x}} \operatorname{tr}_{\mathrm{B}}\left[\Pi\left(E_{\mathbf{x}}\right)^{\circ}\right] \otimes \omega_{\mathrm{B}}\left(E_{\mathbf{x}}\right), \tag{4.1}
\end{equation*}
$$

with $\omega_{\mathrm{B}}\left(E_{\mathbf{x}}\right)=\Pi\left(E_{\mathbf{x}}\right) / v\left(E_{\mathbf{x}}\right)$ and $v\left(E_{\mathbf{x}}\right)=\operatorname{tr}\left[\Pi\left(E_{\mathbf{x}}\right)\right]=\prod_{v} v\left(E_{x_{v}}\right)$, and then using the Nakajima-Zwanzig equation analogously to Sec.3.3.1. For the EMME to have an additive structure with respect to each bath, we have to prove that the crossed correlations of the form

$$
\begin{equation*}
C_{1, v v^{\prime}}\left(E, E^{\prime} ; \tau\right):=\operatorname{tr}_{\mathrm{B}}\left[\delta \tilde{B}_{v}(\tau) \Pi\left(E_{\mathbf{x}}\right) \delta B_{v^{\prime}} \omega_{\mathrm{B}}\left(E_{\mathbf{x}^{\prime}}\right)\right], \tag{4.2}
\end{equation*}
$$

with $v \neq v^{\prime}$ vanish. But this is easy to see since for $v \neq v^{\prime}$, we have

$$
\begin{align*}
C_{1, v v^{\prime}}\left(E, E^{\prime} ; \tau\right): & =\operatorname{tr}_{\mathrm{B}}\left[\delta \tilde{B}_{v}(\tau) \Pi\left(E_{\mathbf{x}}\right) \delta B_{v^{\prime}} \omega_{\mathrm{B}}\left(E_{\mathbf{x}^{\prime}}\right)\right] \\
& =\operatorname{tr}_{v}\left[\delta \tilde{B}_{v}(\tau) \omega_{v}\left(E_{x_{v}}\right)\right] \operatorname{tr}_{v^{\prime}}\left[\delta B_{v^{\prime}} \omega_{v^{\prime}}\left(E_{x_{v^{\prime}}}\right)\right]=0 . \tag{4.3}
\end{align*}
$$

Thus, even though we do not discuss explicitly the thermodynamics with multiple baths, many of the following results can be extended to multiple baths by exploiting the additive structure of the EMME. We refer the interested reader to Ref. [RSS21b] for an extended discussion.

### 4.2 The laws of thermodynamics

The aim of this section is providing a nonequilibrium thermodynamic framework to describe the dynamical evolution of quantum systems in contact with finite baths. Even though our master equation describes a dynamically evolving bath not described by a Gibbs state, we derive the first and second law of thermodynamics as well as the Clausius inequality.

### 4.2.1 The first law of thermodynamics

The first law of thermodynamics essentially states that the energy of an isolated system is conserved. To discuss it, we need to introduce the notions of internal energy work and heat. A natural way to define the (coarse-grained) internal energy of the universe, corresponds to

$$
\begin{equation*}
\mathrm{U}(t):=\sum_{i, x}\left[\varepsilon_{i}\left(\xi_{t}\right)+E_{x}\right] p\left(\varepsilon_{i}, E_{x}\right)=: \mathrm{U}_{\mathrm{S}}+\mathrm{U}_{\mathrm{B}}, \tag{4.4}
\end{equation*}
$$

where $U_{S}$ and $U_{B}$ are the internal energy of the system and the bath, respectively. In Sec. 3.5, we have seen that $\partial_{t} U=0$ under the dynamics generated by the EMME. Hence, the definition in Eq. (4.4) guarantees that in the absence of time-dependent forces the internal energy of the system-bath composite is conserved.

In the presence of a time-dependent system Hamiltonian, the internal energy $U$ can only change due to the mechanical work W done on the system. Hence, using that $\partial_{t} \mathrm{U}=0$, we arrive at the definition for the internal work

$$
\begin{equation*}
\dot{\mathrm{W}}:=\frac{d}{d t} \mathrm{U}=\sum_{k, x}\left[\partial_{t} \varepsilon_{i}\left(\xi_{t}\right)\right] p\left(\varepsilon_{i}, E_{x}\right) \tag{4.5}
\end{equation*}
$$

Since the open quantum system is open; that is, in contact with the finite bath, the change in its internal energy is now due to work and heat. Defining the heat flux as

$$
\begin{equation*}
\dot{\mathrm{Q}}:=-\sum_{i, x} E_{x} \partial_{t} p\left(\varepsilon_{i}, E_{x}\right)=\sum_{i, x} \varepsilon_{i}\left(\xi_{t}\right) \partial_{t} p\left(\varepsilon_{i}, E_{x}\right), \tag{4.6}
\end{equation*}
$$

where the second equality follows again from $\partial_{t} U=0$, we arrive at

$$
\begin{equation*}
\frac{d}{d t} \mathrm{U}_{\mathrm{S}}=\dot{\mathrm{W}}+\dot{\mathrm{Q}} . \tag{4.7}
\end{equation*}
$$

which is a consequence of global energy conservation, and has the usual form of the first law of thermodynamics.

### 4.2.2 The second law of thermodynamics

The second law of thermodynamics states that a change in the thermodynamic entropy of the universe is always non-negative. However, there is no consensus on the microscopic definition of the thermodynamic entropy. Given that we have a probabilistic knowledge of the coarse-grained energy distribution of the isolated system-bath composite, we take the observational entropy $\mathrm{S}_{\mathrm{obs}}^{H_{s}\left(\xi_{s}\right)+\left\{H_{B}\right\}}$ (see Eq. (2.141)) as the proper thermodynamic entropy $S(t)$ at our level of description, in and out of equilibrium. Namely, we define the thermodynamic entropy $\left(k_{\mathrm{B}}=1\right)$ as

$$
\begin{equation*}
\mathrm{S}(t):=\sum_{i, x} p\left(\varepsilon_{i}, E_{x}\right)\left[-\log p\left(\varepsilon_{i}, E_{x}\right)+\log v\left(E_{x}\right)\right] . \tag{4.8}
\end{equation*}
$$

The use of the observational entropy as the thermodynamic entropy has been put forward recently [SDA19b; SDA19a; SŠA20; SW21]. However, it first appearance in quantum thermodynamics can be tracked back to private correspondence between von Neumann and Wigner [Neu10]. Note that, for a diagonal state in the energy
eigenbasis with $\left\langle i, e_{k}\right| \rho\left|i, e_{k}\right\rangle=p\left(\varepsilon_{i}, E_{x}\right) / v\left(E_{x}\right)$ for all $e_{k}$ compatible with $E_{x}$, we find that the observational entropy equals the von Neumann entropy; that is, $\mathrm{S}=\mathrm{S}_{\mathrm{vN}}[\rho]$.

The form of the observational entropy in Eq. (4.8) suggests that it can be rewritten in terms of a "classical" relative entropy which we define as

$$
\begin{equation*}
D^{\mathrm{cl}}(\mathbf{p} \| \mathbf{q}):=\sum_{i, x} p\left(\varepsilon_{i}, E_{x}\right)\left[\log p\left(\varepsilon_{i}, E_{x}\right)-\log q\left(\varepsilon_{i}, E_{x}\right)\right] \geq 0 \tag{4.9}
\end{equation*}
$$

for probability vectors $\mathbf{p}$ and $\mathbf{q}$ at the coarse-grained level of description. Then, it is easy to see that

$$
\begin{equation*}
\mathrm{S}(t)=-D^{\mathrm{cl}}\left(\mathbf{p} \| \mathbf{p}^{\mathrm{st}}\right)+\log \left(d_{\mathrm{S}} d_{\mathrm{B}}\right), \tag{4.10}
\end{equation*}
$$

where the stationary state $p^{\mathrm{st}}\left(\varepsilon_{i}, E_{x}\right)=v\left(E_{x}\right) /\left(d_{\mathrm{S}} d_{\mathrm{B}}\right)$ and $d_{\mathrm{S}}$ and $d_{\mathrm{B}}$ are the system and bath dimensions respectively. Importantly, the stationary state $\mathbf{p}^{\text {st }}$ fulfills the stationary condition (3.75) and is independent of the driving $\xi_{t}$. Then, the quantity $\log d_{\mathrm{S}} d_{\mathrm{B}}$ can be regarded as the maximum entropy.

The second law of thermodynamics stands that the entropy production $\Sigma:=$ $\Delta S(t)=S(t)-S(0)$ is positive for any physically allowed transformation. A more restrictive version of the second law stands that at every time step, the entropy production rate is positive; that is, $\dot{\Sigma}=d \mathrm{~S}(t) / d t \geq 0$. Taking the derivative of Eq. (4.10) we see that

$$
\begin{equation*}
\dot{\Sigma}:=\frac{d}{d t} \mathrm{~S}(t)=-\frac{d}{d t} D^{\mathrm{cl}}\left(\mathbf{p} \| \mathbf{p}^{\mathrm{st}}\right) \tag{4.11}
\end{equation*}
$$

Therefore, proving that the relative entropy $D^{\mathrm{cl}}\left(\mathbf{p} \| \mathbf{p}^{\text {st }}\right)$ decreases monotonically under the evolution equation (3.72) is equivalent to proving that the entropy production rate is always positive.

For compactness, we use for the proof the joint index $n=(i, x)$ so that $p(n)$ denotes the joint probability $p\left(\varepsilon_{i}, E_{x}\right)$ and, also, the ratio $r(n)=p(n) / p^{\text {st }}(n)$. We see that

$$
\begin{align*}
\frac{d}{d t} D^{\mathrm{cl}}\left(\mathbf{p} \| \mathbf{p}^{\text {st }}\right) & =\sum_{n}\left[\partial_{t} p(n)\right]\{\log r(n)+1\} \\
& =\sum_{n n^{\prime}}\left[\Lambda\left(\xi_{t}\right)\right]_{n n^{\prime}} p^{\text {st }}\left(n^{\prime}\right)\left\{r\left(n^{\prime}\right) \log r(n)-r\left(n^{\prime}\right) \log r\left(n^{\prime}\right)\right\}, \tag{4.12}
\end{align*}
$$

where $\Lambda\left(\xi_{t}\right)$ is the possibly driving dependent dynamical matrix for the populations. We now note that, using the stationarity of $\mathbf{p}^{\text {st }}$, the combination

$$
\begin{equation*}
\sum_{n n^{\prime}}\left[\Lambda\left(\xi_{t}\right)\right]_{n n^{\prime}} p^{\mathrm{st}}\left(n^{\prime}\right)\left[\psi(n)-\psi\left(n^{\prime}\right)\right]=0 \tag{4.13}
\end{equation*}
$$

for an arbitrary set of numbers $\{\psi(n)\}$. Let $\psi(n)=r(n)$, and add it to Eq. (4.12) to find at the equation

$$
\begin{equation*}
\frac{d}{d t} D^{\mathrm{cl}}\left(\mathbf{p} \| \mathbf{p}^{\text {st }}\right)=-\sum_{n n^{\prime}}\left[\Lambda\left(\xi_{t}\right)\right]_{n n^{\prime}} p^{\text {st }}\left(n^{\prime}\right) r\left(n^{\prime}\right)\left\{\frac{r(n)}{r\left(n^{\prime}\right)}-\log \frac{r(n)}{r\left(n^{\prime}\right)}-1\right\} \leq 0, \tag{4.14}
\end{equation*}
$$

which is negative since $x \geq 1+\log x$ for all $x \geq 0$ and, therefore, all summands in Eq. (4.14) are positive. Hence, we arrive at the second law

$$
\begin{equation*}
\dot{\Sigma}:=\frac{d}{d t} \mathrm{~S}(t)=-\frac{d}{d t} D^{\mathrm{cl}}\left(\mathbf{p} \| \mathbf{p}^{\mathrm{st}}\right) \geq 0 \tag{4.15}
\end{equation*}
$$

showing that the entropy production rate is always positive under the EMME.
To conclude, the second law follows from two facts: First, $\mathbf{p}^{\text {st }}$ is an equilibrium state of the dynamics and, second, the dynamics of $\mathbf{p}$ are given in the classical master equation form in Eq. (3.73). If any of these two assumptions is violated, negative entropy production rates can appear, although $\Sigma(t)=\Delta \mathrm{S}_{\text {obs }}(t)$ remains positive [SW21].

### 4.2.3 Clausius inequality

We have derived independently the first and second law of thermodynamics and, at this point, they appear rather disconnected. The aim of this subsection is deriving Clausius inequality from our dynamical description based on the EMME. Before proceeding with the derivation, however, we take the opportunity to remind the reader about the phenomenological origin of this inequality.

In standard phenomenological thermodynamics, the first and second law are related through the well-known Clausius inequality. More than 150 years ago, Clausius wrote down the following inequality, which now bears his name [Cla65]:

$$
\begin{equation*}
\Delta \mathrm{S}_{\mathrm{s}}(t)-\int_{0}^{t} \beta\left(t^{\prime}\right) d \mathrm{Q}\left(t^{\prime}\right) \geq 0 \tag{4.16}
\end{equation*}
$$

where $\Delta \mathrm{S}_{\mathrm{S}}(t)$ is the change in thermodynamic entropy of a large system. Clausius had in mind a process where an open system $S$ undergoes a nonequilibrium transformation for a time $t$, while being in contact with an ideal heat bath at a time-dependent inverse temperature $\beta\left(t^{\prime}\right)$ with which it exchanged an infinitesimal amount of heat $d \mathrm{Q}\left(t^{\prime}\right)$ at time $t^{\prime}$. Since an ideal heat bath is characterized by the property $d \mathrm{~S}_{\mathrm{B}}\left(t^{\prime}\right)=\beta\left(t^{\prime}\right) d \mathrm{Q}\left(t^{\prime}\right)$, being $d \mathrm{~S}_{\mathrm{B}}\left(t^{\prime}\right)$ the infinitesimal change in bath entropy, then, if system and bath correlations can be neglected, Eq. (4.16) coincides with the second law $\Delta \mathrm{S}(t) \geq 0$. If the bath is very large, and its temperature remains

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constant during the transformation to its initial value $\beta(0)=\beta_{0}$, then Eq. (4.16) reduces to

$$
\begin{equation*}
\Delta \mathrm{S}_{\mathrm{S}}(t)-\beta_{0} \mathrm{Q}(t) \geq 0, \tag{4.17}
\end{equation*}
$$

where $\mathrm{Q}(t)$ is the total heat exchanged. So far, our considerations are purely based in phenomenological thermodynamics.

In quantum thermodynamics, the task is to derive Eq. (4.16) from an underlying microscopic reversible description, and Eq. (4.17) should arise as its consequence. Interestingly, this is not the usual case in quantum thermodynamics, where Eq. (4.17) is considered as the standard Clausius inequality and second law. As we saw in Sec. 2.6.3, deriving Eq. (4.17) is possible under the assumptions that: (i) the initial state is of the form $\rho(0)=\rho_{\mathrm{S}}(0) \otimes \pi_{\mathrm{B}}\left(\beta_{0}\right)$, (ii) the thermodynamic entropy $S$ is identified as the sum of von Neumann entropies of the system plus the bath $\mathrm{S}_{\mathrm{vN}, \mathrm{S}}+\mathrm{S}_{\mathrm{vN}, \mathrm{B}}$, and (iii) the heat flux $\mathrm{Q}(t)$ is identified with minus the change in energy of the bath; that is, $\mathrm{Q}(t)=-\Delta \mathrm{U}_{\mathrm{B}}(t)$.

The aforementioned derivation of Clausius inequality is remarkable because no approximation is done in the size of the bath. For instance, it holds if the bath is a single spin- $1 / 2$ particle. In that case, while Eq. (4.17) is still a valid inequality, the term $-\beta_{0} Q(t)$ does not correspond to the bath entropy change and, hence, Eq. (4.17) is not a consequence of the second law.

In the present derivation, Clausius inequality is a consequence of the second law Eq. (4.15) using the observational entropy as the thermodynamic entropy, it has the form in Eq. (4.16), and it reduces to (4.17) only in the limit of an infinite heat bath with an infinite heat capacity. We will assume that the initial state is of the form $\rho(0)=\rho_{\mathrm{S}} \otimes \pi_{\mathrm{B}}\left(\beta_{0}\right)$ and argue as follows.

We start from the integrated version of the second law (4.15). The first step is noting that

$$
\begin{equation*}
0 \leq \Delta \mathrm{S}(t)=\Delta \mathrm{S}_{\mathrm{S}}(t)+\Delta \mathrm{S}_{\mathrm{B}}(t)-I_{\mathrm{S}: \mathrm{B}}^{\mathrm{cl}}(\mathbf{p}) \leq \Delta \mathrm{S}_{\mathrm{S}}(t)+\Delta \mathrm{S}_{\mathrm{B}}(t), \tag{4.18}
\end{equation*}
$$

where the system entropy is $\mathrm{S}_{\mathrm{S}}(t):=-\sum_{i} p\left(\varepsilon_{i}\right) \log p\left(\varepsilon_{i}\right)$, and similarly the bath entropy $\mathrm{S}_{\mathrm{B}}(t):=-\sum_{x} p\left(E_{x}\right) \log p\left(E_{x}\right) / v\left(E_{x}\right)$, while the always positive coarse-grained mutual information yields $I_{S: \mathrm{B}}^{\mathrm{cl}}(\mathbf{p})=\sum_{i, x} p\left(\varepsilon_{i}, E_{x}\right)\left[\log p\left(\varepsilon_{i}, E_{x}\right)-\log p\left(\varepsilon_{i}\right)-\log p\left(E_{x}\right)\right]$. The next step is to quantify the change of bath entropy.

In our description, during a general transformation $\rho(0) \mapsto \rho(t)$, the bath generically goes through several nonequilibrium states. For those nonequilibrium states, the inverse temperature $\beta(t)$ appearing in Eq. (4.16) may not even be defined. Hence, to derive the Clausius inequality, we need a notion of temperature out of equilibrium. We bring back the definition of the effective nonequilbrium
inverse temperature $\beta^{\star}(t)$ introduced in Eq. (3.98) Sec. 3.6.3. Namely, given the bath energy distribution $p\left(E_{x}\right)$, we associate to it a temperature $\beta^{\star}(t)$ such that the average energy of the bath is equal to the energy of the coarse-grained thermal state $\pi_{\mathrm{B}}\left(\beta^{\star}(t)\right) \propto \exp \left[-\beta^{\star}(t)\left\{H_{\mathrm{B}}\right\}\right]$. More explicitly, recovering the double bracket notation for classical expectation values of the last chapter

$$
\begin{equation*}
\left\langle\left\langle E_{x}\right\rangle\right\rangle_{p}=\sum_{x} E_{x} p\left(E_{x}\right) \stackrel{!}{=} \sum_{x} E_{x} \frac{v\left(E_{x}\right) \exp \left[-\beta^{\star}(t) E_{x}\right]}{Z_{\mathrm{B}}\left(\beta^{\star}(t)\right)}=\left\langle\left\langle E_{x}\right\rangle\right\rangle_{\beta^{\star}(t)}, \tag{4.19}
\end{equation*}
$$

where the last term can equivalently be written as $\left\langle\left\{H_{\mathrm{B}}\right\}\right\rangle_{\beta^{\star}(t)}=\operatorname{tr}\left[\pi_{\mathrm{B}}\left(\beta^{\star}(t)\right)\left\{H_{\mathrm{B}}\right\}\right]$.
For a thermal distribution $p\left(E_{x} ; \beta\right)=v\left(E_{x}\right) \exp \left(-\beta E_{x}\right) / Z_{\mathrm{B}}(\beta)$, we find the differential property $d p\left(E_{x} ; \beta\right)=-d \beta p\left(E_{x} ; \beta\right) \delta E_{x}(\beta)$ with $\delta E_{x}(\beta)=E_{x}-\left\langle\left\langle E_{x}\right\rangle\right\rangle_{\beta}$. From this differential relation we can easily compute the differential internal energy change

$$
\begin{equation*}
d \mathrm{U}_{\mathrm{B}}=\sum_{x} E_{x} d p\left(E_{x} ; \beta\right)=-d \beta\left\langle\left\langle\delta E_{x}(\beta)^{2}\right\rangle\right\rangle_{\beta}, \tag{4.20}
\end{equation*}
$$

and likewise the differential change of entropy

$$
\begin{equation*}
d \mathrm{~S}_{\mathrm{B}}=\sum_{x} d p\left(E_{x} ; \beta\right)\left[-\log p\left(E_{x} ; \beta\right)+\log v\left(E_{x}\right)-1\right]=-\beta d \beta\left\langle\left\langle\delta E_{x}(\beta)^{2}\right\rangle\right\rangle_{\beta} . \tag{4.21}
\end{equation*}
$$

Combining Eqs. (4.20) and (4.21) we arrive at the well-known relation

$$
\begin{equation*}
d \mathrm{~S}_{\mathrm{B}}=\beta d \mathrm{U}_{\mathrm{B}} \tag{4.22}
\end{equation*}
$$

We use now the assumption that the initial state has the form $\rho(0)=\rho_{\mathrm{S}} \otimes \pi_{\mathrm{B}}\left(\beta_{0}\right)$. With the differential relation in Eq. (4.22), we can rewrite any change in bath entropy as

$$
\begin{align*}
\Delta \mathrm{S}_{\mathrm{B}}(t) & =\mathrm{S}_{\mathrm{B}}(t)-\mathrm{S}_{\mathrm{B}}\left[\pi_{\mathrm{B}}\left(\beta^{\star}(t)\right)\right]+\mathrm{S}_{\mathrm{B}}\left[\pi_{\mathrm{B}}\left(\beta^{\star}(t)\right)\right]-\mathrm{S}_{\mathrm{B}}(0) \\
& =\mathrm{S}_{\mathrm{B}}(t)-\mathrm{S}_{\mathrm{B}}\left[\pi_{\mathrm{B}}\left(\beta^{\star}(t)\right)\right]+\int_{0}^{t} d t^{\prime} \beta^{\star}\left(t^{\prime}\right) d \mathrm{U}_{\mathrm{B}}\left(t^{\prime}\right) . \tag{4.23}
\end{align*}
$$

We are now ready to derive the Clausius inequality. The next step is to use Eq. (4.23) together with the property that, given average energy $\mathrm{U}_{\mathrm{B}}(t)$, the thermal state is that of larger entropy. Then,

$$
\begin{equation*}
\Delta \mathrm{S}_{\mathrm{S}}(t)+\Delta \mathrm{S}_{\mathrm{B}}(t) \leq \Delta \mathrm{S}_{\mathrm{S}}(t)-\int_{0}^{t} d t^{\prime} \beta^{\star}\left(t^{\prime}\right) \dot{\mathrm{Q}}\left(t^{\prime}\right) \tag{4.24}
\end{equation*}
$$

where we have identified $d \mathrm{U}_{\mathrm{B}}(t)=-\dot{\mathrm{Q}}(t) d t$. Finally, in the limit of an infinite bath, when the extensive heat capacity tends to infinity, the nonequilibrium effective
inverse temperature $\beta^{\star}(t)=\beta_{0}$ remains constant during the transformation (see Eq. (3.99)). Then, putting everything together, we find the hierarchy of second laws

$$
\begin{align*}
0 & \leq \Delta \mathrm{S}(t) \\
& \leq \Delta \mathrm{S}_{\mathrm{S}}(t)+\Delta \mathrm{S}_{\mathrm{B}}(t) \\
& \leq \Delta \mathrm{S}_{\mathrm{S}}(t)-\int_{0}^{t} d t^{\prime} \beta^{\star}\left(t^{\prime}\right) d \mathrm{Q}\left(t^{\prime}\right) \\
& \leq \Delta \mathrm{S}_{\mathrm{S}}(t)-\beta_{0} \mathrm{Q}(t) . \tag{4.25}
\end{align*}
$$

which reproduce, in the appropriate limit, the phenomenological Clausius inequality. As a final remark, we note that the second inequality becomes an equality when the bath does not develop nonequilibrium features.

### 4.3 Example: Driven Random Matrix Bath Model

We recover now the random matrix model studied in Sec. 3.4. We slightly generalize it in the following sense. First, we allow the system Hamiltonian to depend on time as $H_{\mathrm{S}} \mapsto H_{\mathrm{S}}\left(\xi_{t}\right)=\xi_{t} \omega_{0} \sigma_{0}^{z} / 2$, and we chose $\omega_{0}=2 \delta E$. The driving protocol is specified as

$$
\xi_{t}=\left\{\begin{array}{cc}
1 & \text { for } t \in\left[0, \tau_{\mathrm{d}} / 2\right)  \tag{4.26}\\
2 & \text { for } t \in\left[\tau_{\mathrm{d}} / 2, \tau_{\mathrm{d}}\right)
\end{array}\right.
$$

and repeats periodically with the driving period $\tau_{\mathrm{d}}$; that is, $\xi_{t+\tau_{\mathrm{d}}}=\xi_{t}$. In this case, we consider that the driving is slow if the relaxation time of the bath is fast as compared to the driving period; that is, $\tau_{\mathrm{B}} \ll \tau_{\mathrm{d}}$. Second, we assume that a third energy band is present, so that the coarse-grained description of the bath is

$$
\begin{equation*}
\left\{H_{\mathrm{B}}\right\}=\delta E\left[-\Pi\left(E_{-}\right)+\Pi\left(E_{+}\right)+3 \Pi\left(E_{3}\right)\right], \tag{4.27}
\end{equation*}
$$

so that the transition $E_{3}-E_{-}=4 \delta E$ becomes equal to $2 \omega_{0}$. We take the bath interaction to be given by the random operator

$$
\begin{equation*}
B=\sum_{e_{k} \in E_{+}, E_{3}} \sum_{e_{q} \in E_{-}} B_{k q}\left|e_{k} X e_{q}\right|+\text { h.c. } \tag{4.28}
\end{equation*}
$$

and with the same stochastic properties than in Sec. 3.4.
We assume that initially, the system-bath composite is found in the state $\rho(0)=|+X+| \otimes \omega_{\mathrm{B}}\left(E_{-}\right)$. Following Sec. 3.4, we see that there are three probabilities that enter the dynamics. We gather them in the probability vector $\mathbf{p}=$


Figure 4.1: Dynamics and thermodynamics of a driven spin- $1 / 2$ particle subject to the driving $\xi_{t}$. White background corresponds to $\xi_{t}=1$, while gray background corresponds to $\xi_{t}=2$ (see main text for details). (Top-left) Comparison of the exact dynamics (circle, triangle and diamond markers) with the dynamics predicted by the time-local equation (solid, dashed and dotted lines) for the three non-zero probabilities $p\left(\varepsilon_{i}, E_{x}\right)$; (top-right) evolution of the effective nonequilibrium inverse temperature $\beta^{\star}(t)$; (bottom-left) dynamics of the quantities contributing to the first law: (solid orange line) system internal energy, (dashed blue line) heat, and (yellow dotted line) work; (bottom-right) hierarchy of second laws: total change in observational entropy (solid orange line), system plus bath change in observational entropy (blue dashed line), and the LHS of Clausius inequality (4.19). The initial state is $\rho(0)=|+X+| \otimes \omega_{\mathrm{B}}\left(E_{-}\right)$. The parameters are taken as $\omega_{0}=2 \delta E, v\left(E_{-}\right)=100$, $v\left(E_{+}\right)=200, v\left(E_{3}\right)=400, \lambda=0.01 \delta E$, and $\tau_{d}=50 \delta E^{-1}$.
$\left[p\left(\varepsilon_{-}, E_{+}\right), p\left(\varepsilon_{+}, E_{-}\right), p\left(\varepsilon_{-}, E_{3}\right)\right]^{T}$. In the subspace of the first two components, the dynamical matrix for $t \in\left[0, \tau_{\mathrm{d}} / 2\right)$ is identical to Eq. (3.59) and zero elsewhere; that is,

$$
\Lambda\left(\xi_{t}\right)=\frac{2 \pi \lambda^{2}}{\delta E}\left(\begin{array}{ccc}
-v\left(E_{-}\right) & v\left(E_{+}\right) & 0  \tag{4.29}\\
v\left(E_{-}\right) & -v\left(E_{+}\right) & 0 \\
0 & 0 & 0
\end{array}\right) \quad \text { for } t \in\left[0, \tau_{\mathrm{d}} / 2\right)
$$

Instead, for $t \in\left[\tau_{\mathrm{d}} / 2, \tau_{\mathrm{d}}\right)$, we have the dynamical matrix

$$
\Lambda\left(\xi_{t}\right)=\frac{2 \pi \lambda^{2}}{\delta E}\left(\begin{array}{ccc}
0 & 0 & 0  \tag{4.30}\\
0 & -v\left(E_{3}\right) & v\left(E_{-}\right) \\
0 & v\left(E_{3}\right) & -v\left(E_{-}\right)
\end{array}\right) \quad \text { for } t \in\left[\tau_{\mathrm{d}} / 2, \tau_{\mathrm{d}}\right)
$$

In the top-left panel of Fig. 4.1, we compare the exact dynamics of the present driven random matrix bath model (shown with circle, triangle, and diamond markers) with the prediction of the time-local version of the EMME (3.16) (shown with solid, dashed, and dotted lines). We observe that we are able to reproduce accurately the dynamics, even when the system energy levels are periodically quenched. This justifies in retrospective our claim above that we can replace the static system energies $\varepsilon_{i}$ with time-dependent energies $\varepsilon_{i}\left(\xi_{t}\right)$ as long as $\tau_{\mathrm{d}}$ varies slowly compared with the relaxation time of the bath $\tau_{\mathrm{B}}$.

In the top-right panel of Fig. 4.1, we show the evolution of the nonequilibrium effective inverse temperature $\beta^{\star}(t)$. Clearly, the dynamics of this object is not negligible in the model under scrutiny. This fact signals that the thermodynamic properties of the driven random matrix bath model cannot be treated with the conventional infinite bath thermodynamic framework.

In the bottom-row of Fig. 4.1, we show the first and second law for the driven random matrix bath model. In the bottom-left panel, we show the evolution of the system internal energy (solid orange line), the heat exchanged with the finite bath (dashed blue line), and the work exchanged with the driving (yellow dotted line). As expected, work is introduced or extracted from the system only when the driving $\xi_{t}$ changes its value. In the bottom-right panel, we compare the different second laws in Eq. (4.25). The solid orange line corresponds to the change in observational entropy of the system bath composite, which increases monotonously. Ignoring the system bath correlations contained in the mutual information $I_{\mathrm{S}: \mathrm{B}}^{\mathrm{cl}}$, one obtains a less tight bound, that corresponds to adding up the system and the bath contributions to the observational entropy (blue dashed line). Finally, if one disregards the nonequilibrium transformations in the bath, one obtains an even less tight bound corresponding to the Clausius inequality (yellow dotted line). The
version of Clausius inequality at the initial inverse temperature $\beta_{0}$ is not shown in the figure.

### 4.4 General relation between entropy productions

In Sec. 4.2.3, we have discussed that Clausius inequality in its original form (4.16) is the appropriate inequality to discuss the entropy production of an open quantum system coupled to a finite bath. The microscopically derived version of Eq. (4.16) appearing in Eq. (4.25) is valid even out of equilibrium and does not rely on the Gibbs state. Instead, the inequality Eq. (4.17) should be used only when the heat capacity of the bath is infinite, at least at a practical level. As we shall see, using Eq. (4.16) instead of Eq. (4.17), reveals surprising insights for finite-time information erasure and heat engines, which have higher efficiencies than previously thought.

### 4.4.1 General discussion

Consider an open quantum system that is coupled to a potentially finite bath, from which we have only coarse-grained knowledge about its energy distribution. Initially, the system-bath composite is found in the state $\rho(0)=\rho_{\mathrm{S}}(0) \otimes \pi_{\mathrm{B}}\left(\beta_{0}\right)$, being the Gibbs state $\pi_{\mathrm{B}}\left(\beta_{0}\right) \propto \exp \left(-\beta_{0}\left\{H_{\mathrm{B}}\right\}\right)$, defined according to the coarse-grained Hamiltonian. For the sake of the discussion, we introduce two different entropy productions $\Sigma$ and $\Sigma^{\prime}$ associated with a transformation process $\rho(0) \mapsto \rho(t)$. They correspond to the independent Clausius inequalities

$$
\begin{align*}
& \Sigma(t)=\Delta \mathrm{S}_{\mathrm{S}}(t)-\int_{0}^{t} d t^{\prime} \beta^{\star}\left(t^{\prime}\right) \dot{\mathrm{Q}}\left(t^{\prime}\right) \geq 0  \tag{4.31}\\
& \Sigma^{\prime}(t)=\Delta \mathrm{S}_{\mathrm{S}}(t)-\beta_{0} \mathrm{Q}(t) \geq 0 \tag{4.32}
\end{align*}
$$

where the quantities entering both inequalities have the same microscopic definitions.

A natural question arise: is there a definite relation between $\Sigma(t)$ and $\Sigma^{\prime}(t)$ ? The answer is positive, and is simply found by subtracting $\Sigma(t)$ from $\Sigma^{\prime}(t)$ and manipulating the result. We note that

$$
\begin{equation*}
\Sigma^{\prime}(t)-\Sigma(t)=-\beta_{0} \mathrm{Q}(t)-\mathrm{S}_{\mathrm{B}}\left(\tau_{\mathrm{B}}\left(\beta^{\star}(t)\right)\right)+\mathrm{S}_{\mathrm{B}}\left(\tau_{\mathrm{B}}\left(\beta_{0}\right)\right) . \tag{4.33}
\end{equation*}
$$

Next, we rewrite the total heat exchanged as

$$
\begin{equation*}
-\beta_{0} \mathrm{Q}(t)=\operatorname{tr}\left[\rho_{\mathrm{B}}(t)-\pi\left(\beta_{0}\right)\right] \log \pi_{\mathrm{B}}\left[\beta_{0}\right] . \tag{4.34}
\end{equation*}
$$

However, we have fixed $\beta^{\star}(t)$ such that $\operatorname{tr}\left[\rho_{\mathrm{B}}(t)\left\{H_{\mathrm{B}}\right\}\right]=\operatorname{tr}\left[\pi\left(\beta^{\star}(t)\right)\left\{H_{\mathrm{B}}\right\}\right]$. Hence,

$$
\begin{equation*}
-\beta_{0} \mathrm{Q}(t)=\operatorname{tr}\left[\rho_{\mathrm{B}}(t)-\pi\left(\beta_{0}\right)\right] \log \pi_{\mathrm{B}}\left[\beta_{0}\right]=\operatorname{tr}\left[\pi_{\mathrm{B}}\left(\beta^{\star}(t)\right)-\pi\left(\beta_{0}\right)\right] \log \pi_{\mathrm{B}}\left[\beta_{0}\right] . \tag{4.35}
\end{equation*}
$$

Combining Eqs. (4.33) and (4.35), we arrive at the relation

$$
\begin{equation*}
\Sigma^{\prime}(t)-\Sigma(t)=D\left(\pi\left[\beta^{\star}(t)\right] \| \pi\left[\beta_{0}\right]\right) \geq 0 . \tag{4.36}
\end{equation*}
$$

The central result (4.36) tells us that the entropy production $\Sigma(t)$ is smaller than what one would naively expect from $\Sigma^{\prime}(t)$. Thus, physical transformations of physical systems in contact with finite baths are less irreversible if one considers the entropy production $\Sigma$. Physically speaking, we can explain Eq. (4.36) by pointing out that the available information about the heat flow $\mathrm{Q}(t)$ is taken fully into account in $\Sigma$ but only partially in $\Sigma^{\prime}$. The inequality $\Sigma^{\prime}(t) \geq 0$ reflects the second law for an observer who ignores that the bath is finite. However, if one already knows the heat flow $\mathrm{Q}(t)$, one can use it to gain a more accurate description via the definition of the effective nonequilibrium inverse temperature $\beta^{\star}(t)$ in Eq. (4.19). Thus, $\Sigma$ efficiently uses the available information and the loss in predictive power resulting from ignoring the finiteness of the bath is quantified by the relative entropy in Eq. (4.36). Remarkably, since the effective temperature $\beta^{\star}(t)$ is in one-to-one correspondence to the bath energy, Eq. (4.36) also reveals that the computation of $\Sigma$ does not require more information than the computation of $\Sigma^{\prime}$ : both are uniquely fixed by knowing $\beta_{0}$ and $\mathrm{Q}\left(t^{\prime}\right)$.

Another interpretation of Eq. (4.36) is the following. Suppose that we have an additional infinitely large superbath at our disposal with fixed temperature $\beta_{0}$. After the finite bath has interacted with the system, it is out of equilibrium with respect to this superbath if $\beta^{\star}(t) \neq \beta_{0}$. This nonequilibrium situation can be used to extract work. The maximum extractable work equals the change in free energy: $\mathrm{W}_{\text {ext }}^{\max }=$ $\mathrm{F}_{\mathrm{B}}\left(\beta^{\star}(t)\right)-\mathrm{F}_{\mathrm{B}}\left(\beta_{0}\right)\left[\mathrm{BCG}+19 ;\right.$ LP20]. Here, $\mathrm{F}_{\mathrm{B}}\left(\beta^{\star}(t)\right):=\mathrm{U}_{\mathrm{B}}(t)-\beta_{0}^{-1} \mathrm{~S}_{\mathrm{vN}, \mathrm{B}}\left(\beta^{\star}(t)\right)$ denotes the nonequilibrium free energy with respect to the reference inverse temperature $\beta_{0}$. Note that, even if $\rho_{\mathrm{B}}(t) \neq \pi_{\mathrm{B}}\left[\beta^{\star}(t)\right], \mathrm{F}_{\mathrm{B}}\left(\beta^{\star}(t)\right)$ correctly quantifies the nonequilibrium free energy at time $t$ based on our level of description, which assumes only the bath energy to be known (in case of additional information, more work can be extracted). We find

$$
\begin{equation*}
\mathrm{W}_{\mathrm{ext}}^{\max }(t)=\beta_{0}^{-1}\left[\Sigma^{\prime}(t)-\Sigma(t)\right] \geq 0 . \tag{4.37}
\end{equation*}
$$

Thus, if we demand that the bath in our description gets reset after each process to its initial temperature, Eq. (4.36) tells us that we can always use this reset stage to extract useful work, which remains unaccounted for in Eq. (4.32). In the following, we explicitly demonstrate the use and benefit of Eq. (4.31) for heat engines.

### 4.4.2 Multiple heat baths and stationary regime

For some practical applications, for instance thermal machines, one has to consider multiple heat baths. We consider that the initial state is given by $\rho(0)=$ $\rho_{\mathrm{S}}(0) \otimes_{v} \pi_{v}\left(\beta_{0, v}\right)$. Then, the analysis of the previous section holds also for multiple finite baths. The two entropy productions are, in this case

$$
\begin{align*}
& \Sigma(t)=\Delta \mathrm{S}_{\mathrm{S}}(t)-\sum_{v} \int_{0}^{t} d t^{\prime} \beta_{v}^{\star}\left(t^{\prime}\right) \dot{\mathrm{Q}}_{v}\left(t^{\prime}\right) \geq 0,  \tag{4.38}\\
& \Sigma^{\prime}(t)=\Delta \mathrm{S}_{\mathrm{S}}(t)-\sum_{v} \beta_{0, v} \mathrm{Q}_{v}(t) \geq 0, \tag{4.39}
\end{align*}
$$

where $v$ labels the possibly multiple finite baths. Now, arguing analogously to the previous section, we conclude that

$$
\begin{equation*}
\Sigma^{\prime}(t)-\Sigma(t)=\sum_{v} D^{\mathrm{qm}}\left(\pi_{v}\left(\beta_{v}^{\star}(t)\right) \| \pi_{v}\left(\beta_{0, v}\right)\right) \geq 0 \tag{4.40}
\end{equation*}
$$

Often, thermal machines operate cyclically for long periods of time. For simplicity, we assume that the engine has operated for a sufficient amount of time (or cycles) such that its change in entropy $\Delta \mathrm{S}_{\mathrm{S}}$ and internal energy $\Delta \mathrm{U}_{\mathrm{S}}$ is negligible compared to other terms appearing in the first and second law. This is called the stationary regime, and it is well justified if the system is small in comparison with the baths. Then, it is justified to approximate the first law by

$$
\begin{equation*}
0=\mathrm{W}(t)+\sum_{v} \mathrm{Q}_{v}(t) \tag{4.41}
\end{equation*}
$$

and the two Clausius inequalities as

$$
\begin{align*}
& \Sigma(t)=-\sum_{v} \int_{0}^{t} d t^{\prime} \beta_{v}^{\star}\left(t^{\prime}\right) \dot{\mathrm{Q}}_{v}\left(t^{\prime}\right) \geq 0  \tag{4.42}\\
& \Sigma^{\prime}(t)=-\sum_{v} \beta_{0, v} \mathrm{Q}_{v}(t) \geq 0 \tag{4.43}
\end{align*}
$$

In the following subsection, we make use of such stationary regime to discuss the efficiency of heat engines coupled to finite baths.

### 4.4.3 Heat engines and efficiencies

We consider a heat engine that operates at the stationary regime between two heat sources that correspond to finite baths, and we label by $v=\mathrm{h}, \mathrm{c}$ for hot and cold.

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They are initialized at the inverse temperatures $\beta_{0, \mathrm{~h}} \leq \beta_{0, \mathrm{c}}$, and we are interested in the efficiency $\eta$.

However, defining an efficiency in the case of finite baths with dynamically evolving temperatures is subtle and requires some care. For work extraction, the standard choice of efficiency is $-\mathrm{W}(t) / \mathrm{Q}_{\mathrm{h}}(t)$, which implies the Carnot bound $\eta_{\mathrm{C}}\left(\beta_{0, \mathrm{~h}}, \beta_{0, \mathrm{c}}\right)=1-\beta_{0, \mathrm{~h}} / \beta_{0, \mathrm{c}}$, is well suited to describe the situation of an engine operating between two heat baths that operate at a fixed temperature. Importantly, this is not the case we are interested in. We define efficiency in the following way.

In general, an efficiency quantifies how much of a certain quantity of interest $A$ we can extract given a certain dynamical constraint in the form of an inequality $\Sigma=\mathrm{A}+\mathrm{B} \geq 0$, for instance the second law. In our sign convention, extracting is reflected with a negative value of the quantity of interest; that is, extracting $A$ it implies $A<0$. Thus, in order to extract $A$ the remaining part $B$ of the entropy production has to "overcompensate" for it in such a way that $\Sigma \geq 0$ remains positive. Then, $\eta=-\mathrm{A} / \mathrm{B} \leq 1$ always defines an efficiency which is bounded by the value $\eta=1$.

In the case of heat engines and work extraction in the stationary regime, our dynamical constraints are given by the first law (4.41) and second law given by either Eq. (4.42) or and (4.43). Hence, for the same physical transformation, two different efficiencies can be defined corresponding to $\Sigma$ and $\Sigma^{\prime}$. First, consider $\Sigma^{\prime}$

$$
\begin{equation*}
\Sigma^{\prime}(t)=-\beta_{0, \mathrm{c}} \mathrm{Q}_{\mathrm{c}}(t)-\beta_{0, h} \mathrm{Q}_{\mathrm{h}}(t)=\beta_{0, \mathrm{c}}\left[\mathrm{~W}(t)+\mathrm{Q}_{\mathrm{h}}(t)\right]-\beta_{0, h} \mathrm{Q}_{\mathrm{h}}(t) \geq 0, \tag{4.44}
\end{equation*}
$$

where we have used Eq. (4.41) to rewrite $\mathrm{Q}_{\mathrm{c}}$ in terms of $\mathrm{W}(t)$ and $\mathrm{Q}_{\mathrm{h}}$. We identify the quantities $\mathrm{A}(t)=\beta_{0, \mathrm{c}} \mathrm{W}(t)$ and $\mathrm{B}^{\prime}(t)=\left[\beta_{0, \mathrm{c}}-\beta_{0, \mathrm{~h}}\right] \mathrm{Q}_{\mathrm{h}}(t)$. Hence, applying the aforementioned logic we obtain

$$
\begin{equation*}
\eta^{\prime}(t)=-\frac{\mathrm{A}(t)}{\mathrm{B}^{\prime}(t)}=\frac{\beta_{0, \mathrm{c}}}{\beta_{0, \mathrm{c}}-\beta_{0, \mathrm{~h}}} \frac{-\mathrm{W}(t)}{\mathrm{Q}_{\mathrm{h}}(t)}=\frac{1}{\eta_{\mathrm{c}}\left(\beta_{0, \mathrm{~h}}, \beta_{0, \mathrm{c}}\right)} \frac{-\mathrm{W}(t)}{\mathrm{Q}_{\mathrm{h}}(t)} \leq 1 \tag{4.4}
\end{equation*}
$$

which is just a rescaled version of Carnot efficiency such that is bounded by 1 .
Instead, if we consider the dynamical constraint $\Sigma$, we have

$$
\begin{equation*}
\Sigma(t)=\Sigma^{\prime}(t)+\left[\Sigma(t)-\Sigma^{\prime}(t)\right]=\mathrm{A}(t)+\mathrm{B}^{\prime}(t)+\left[\Sigma(t)-\Sigma^{\prime}(t)\right] \geq 0, \tag{4.46}
\end{equation*}
$$

from which we identify $B(t)=B^{\prime}(t)+\left[\Sigma(t)-\Sigma^{\prime}(t)\right]$. Therefore, if we define the efficiency

$$
\begin{equation*}
\eta(t)=-\frac{\mathrm{A}(t)}{\mathrm{B}(t)}=-\frac{\mathrm{A}(t)}{\mathrm{B}^{\prime}(t)} \frac{\mathrm{B}^{\prime}(t)}{\mathrm{B}(t)}=\frac{1}{1+\frac{\Sigma(t)-\Sigma^{\prime}(t)}{\eta_{\mathrm{C}}\left(\beta_{0, \mathrm{~h}} \beta_{0, c}\right) \beta_{0, c} \mathrm{C}_{\mathrm{h}}(t)}} \eta^{\prime}(t) . \tag{4.47}
\end{equation*}
$$

The denominator of Eq. (4.47) is smaller than one, which leads to $\eta(t) \geq \eta^{\prime}(t)$. This result implies that quantum thermal machines in contact with finite bath have higher efficiencies than previously anticipated. Accordingly, the physical process undergone by the thermal machine is less irreversible if the entropy production is computed with the Clausius inequality (4.38) for finite baths.

To conclude this section, we remark that the stationary regime is not crucial to arrive at the conclusion that thermal machines have a higher efficiency than previously anticipated. A discussion about the non-stationary regime can be found in the supplemental material of Ref. [SDR21b]. To illustrate the above discussion, we introduce a model for the heat engine that combines the SWAP engine with the idea of repeated interactions in the following section.

### 4.5 Example: the SWAP engine

We consider the system $S$ to be a spin- $1 / 2$ particle that interacts with an ideal infinite cold bath and a finite hot bath at inverse temperatures $\beta_{0, \mathrm{c}} \geq \beta_{0, \mathrm{~h}}$, respectively. The system is microscopically described by the Hamiltonian

$$
\begin{equation*}
H_{\mathrm{S}}=\omega_{0} \sigma_{0}^{z} / 2 \tag{4.48}
\end{equation*}
$$

and we denote by $| \pm\rangle$ the energy eigenbasis, which fulfills $H_{\mathrm{S}}| \pm\rangle= \pm \omega_{0} / 2| \pm\rangle$.
We model the cold bath as an ideal bath weakly coupled to the system, which after interacting with the system simply prepares the system in the Gibbs state $\pi_{\mathrm{s}}\left(\beta_{0, \mathrm{c}}\right)=\exp \left(-\beta_{0, \mathrm{c}} H_{\mathrm{S}}\right) / Z_{\mathrm{S}}\left(\beta_{0, \mathrm{c}} \mathrm{c}\right.$, with $Z_{\mathrm{S}}\left(\beta_{0, \mathrm{c}}\right)=\operatorname{tr}\left[\exp \left(-\beta_{0, \mathrm{c}} H_{\mathrm{S}}\right)\right]$.

The hot bath is made out of $N_{s}$ identical and non-interacting spins, and it is microscopically described by the Hamiltonian

$$
\begin{equation*}
H_{\mathrm{h}}=\sum_{r} H_{r}=\sum_{r} \Omega_{\mathrm{h}} \sigma_{r}^{z} / 2 . \tag{4.49}
\end{equation*}
$$

Similarly to the system Hamiltonian, we introduce the states $\left.\left.\right|_{ \pm}\right\rangle_{r}$ which fulfill $H_{\mathrm{h}, r}| \pm\rangle_{r}=\left( \pm \Omega_{\mathrm{h}} / 2\right)| \pm\rangle_{r}$.

We now consider the framework of repeated interactions [SSB+17]. Namely, we consider that at regular times $t_{n}=n \tau_{\mathrm{d}}$, being $\tau_{\mathrm{d}}$ the driving period, the $n^{\text {th }}$ spin of the hot bath interacts with the system. This interaction is assumed to happen instantaneously, which in practice means much faster than any other timescale of the model. Moreover, we assume the time in between interactions $\tau_{\mathrm{d}}$ to be large enough for the system to relax to the equilibrium state $\pi_{\mathrm{s}}\left(\beta_{0, \mathrm{c}}\right)$. Finally, we consider


Figure 4.2: Sketch of our SWAP engine model. A finite hot bath in red (right) and an ideal infinite bath in blue (left) interact alternatively with the spin- $1 / 2$ system (center). The SWAP engine operates in two steps. First, the state of the system is swapped with the state of a spin- $1 / 2$ particle in the finite hot bath. Second, the system thermalizes with the cold bath.
that the interaction between the system and the hot bath implements a SWAP operation $U_{\text {SWAP }}$ in such a way that

$$
\begin{equation*}
U_{\mathrm{SWAP}}|i\rangle_{\mathrm{S}}|k\rangle_{n}=|k\rangle_{\mathrm{S}}|i\rangle_{n} \tag{4.50}
\end{equation*}
$$

for $i, k= \pm$. This model is known as the SWAP engine and was introduced in Ref. [CPF15]. We remark that the effective SWAP interaction has to be thought as a time-dependent Hamiltonian $H_{\text {SWAP }}(t)$ which at a time $t_{n}^{-}$a certain interaction with the $n^{\text {th }}$ is turned on and at a time $t_{n}^{+}$turned off again, in such a way that the corresponding unitary implements a SWAP operation. From a thermodynamic point of view, this time-dependent interaction gives rise to a work contribution at every time $t_{n}$. This SWAP engine is sketched in Fig. 4.2.

We can now start to analyze this model from a thermodynamic perspective. We start by computing the amount of work exchanged in every interaction. Right before and right after the interaction, at times $t_{n}^{-}$and $t_{n}^{+}$, the state of the system is given by

$$
\begin{align*}
& \rho\left(t_{n}^{-}\right)=\pi_{\mathrm{c}}\left(\beta_{0, \mathrm{c}}\right) \otimes \pi_{\mathrm{s}}\left(\beta_{0, \mathrm{c}}\right) \bigotimes_{r=1}^{n-1} \tilde{\pi}_{r}\left(\beta_{0, \mathrm{c}}\right) \bigotimes_{r=n}^{N_{s}} \pi_{r}\left(\beta_{0, \mathrm{~h}}\right),  \tag{4.51}\\
& \rho\left(t_{n}^{+}\right)=\pi_{\mathrm{c}}\left(\beta_{0, \mathrm{c}}\right) \otimes \tilde{\pi}_{\mathrm{S}}\left(\beta_{0, \mathrm{c}}\right) \bigotimes_{r=1}^{n} \tilde{\pi}_{r}\left(\beta_{0, \mathrm{c}}\right) \bigotimes_{r=n+1}^{N_{s}} \pi_{r}\left(\beta_{0, \mathrm{~h}}\right), \tag{4.52}
\end{align*}
$$

being $\tilde{\pi}_{\mathrm{S}}(\beta)=\sum_{i} \exp \left(i \beta \Omega_{\mathrm{h}}\right)\left|i X_{i}\right| / Z_{\mathrm{B}}(\beta)$ and $\tilde{\pi}_{r}(\beta)=\sum_{k} \exp \left(k \beta \omega_{0}\right)|k X k| / Z_{\mathrm{S}}(\beta)$ the "swapped" thermal states. Hence, using the first law (4.5) the work contribution at time $t_{n}$ is given by

$$
\begin{equation*}
d \mathrm{~W}\left(t_{n}\right)=\left(\frac{\omega_{0}}{2}-\frac{\Omega_{\mathrm{h}}}{2}\right)\left[\tanh \left(\frac{\beta_{0, \mathrm{c}} \omega_{0}}{2}\right)-\tanh \left(\frac{\beta_{0, \mathrm{~h}} \Omega_{\mathrm{h}}}{2}\right)\right] . \tag{4.53}
\end{equation*}
$$

where we use the differential notation to denote that the work exchange happens only during the infinitesimal time $t_{n}^{+}-t_{n}^{-}$. From Eq. (4.53), we see that the condition of work extraction $\mathrm{W}\left(t_{n}\right)<0$ requires being in the regime

$$
\begin{equation*}
\frac{\beta_{0, \mathrm{c}}}{\beta_{0, \mathrm{~h}}}>\frac{\Omega_{\mathrm{h}}}{\omega_{0}}>1 . \tag{4.54}
\end{equation*}
$$

Similarly, one can compute also the change in system and bath internal energy during the SWAP operation, which amounts to

$$
\begin{align*}
& d \mathrm{U}_{\mathrm{S}}\left(t_{n}\right)=\frac{\omega_{0}}{2}\left[\tanh \left(\frac{\beta_{0, \mathrm{c}} \omega_{0}}{2}\right)-\tanh \left(\frac{\beta_{0, \mathrm{~h}} \Omega_{\mathrm{h}}}{2}\right)\right]=: \Delta u  \tag{4.55}\\
& d \mathrm{Q}_{\mathrm{h}}\left(t_{n}\right)=-d \mathrm{U}_{\mathrm{h}}\left(t_{n}\right)=\frac{\Omega_{\mathrm{h}}}{2}\left[\tanh \left(\frac{\beta_{0, \mathrm{c}} \omega_{0}}{2}\right)-\tanh \left(\frac{\beta_{0, \mathrm{~h}} \Omega_{\mathrm{h}}}{2}\right)\right]=\frac{\Omega_{\mathrm{h}}}{\omega_{0}} \Delta u, \tag{4.56}
\end{align*}
$$



Figure 4.3: (left) Comparison of the two entropy productions $\Sigma$ (solid orange line) and $\Sigma^{\prime}$ (dashed blue line) in Eqs. (4.58) and (4.59) for the SWAP engine described in the main text; (right) corresponding efficiencies $\eta$ (solid orange line) and $\eta^{\prime}$ (dashed blue line). The parameters are $\Omega_{h}=3 / 2 \omega_{0}, \beta_{0, \mathrm{c}}=3 \omega_{0}^{-1}, \beta_{0, \mathrm{~h}}=\omega_{0}^{-1}$, and $N_{s}=100$.
where $\Delta u$ is the energy gained by the system during the SWAP operation. As expected, the first law is fulfilled during the SWAP operation since $d \mathrm{U}_{\mathrm{S}}\left(t_{n}\right)=$ $d \mathrm{Q}_{\mathrm{h}}\left(t_{n}\right)+d \mathrm{~W}\left(t_{n}\right)$.

During the subsequent equilibration step of duration $\tau_{\mathrm{d}}$, the system at state $\tilde{\pi}_{\mathrm{s}}\left(\beta_{0, \mathrm{~h}}\right)$ relaxes to $\pi_{\mathrm{s}}\left(\beta_{0, \mathrm{c}}\right)$ by releasing the internal energy

$$
\begin{equation*}
\mathrm{U}_{\mathrm{S}}\left(t_{n+1}^{-}\right)-\mathrm{U}_{\mathrm{S}}\left(t_{n}^{+}\right)=-\frac{\omega_{0}}{2}\left[\tanh \left(\frac{\beta_{0, \mathrm{c}} \omega_{0}}{2}\right)-\tanh \left(\frac{\beta_{0, \mathrm{~h}} \Omega_{\mathrm{h}}}{2}\right)\right]=-\Delta u, \tag{4.57}
\end{equation*}
$$

to the cold bath in the form of heat, which concludes the cycle for the state of the system.

In our heat engine model, the amount of heat and work exchanged with the heat baths does not depend on the number of cycles $n$ that have occurred. Hence, we can rewrite the energy balance in terms of absolute quantities as $\mathrm{Q}_{\mathrm{c}}\left(t_{n+1}^{-}\right)=-n \Delta u$, $\mathrm{Q}_{\mathrm{h}}\left(t_{n}^{+}\right)=n \Delta u \Omega_{\mathrm{h}} / \omega_{0}$, and $\mathrm{W}\left(t_{n}^{+}\right)=n\left(1-\Omega_{\mathrm{h}} / \omega_{0}\right) \Delta u$. Therefore, we arrive at the expressions

$$
\begin{align*}
& \Sigma\left(t_{n+1}^{-}\right)=-n \beta_{0, \mathrm{c}} \Delta u+\sum_{r=1}^{n} \beta_{\mathrm{h}}^{\star}\left(t_{n}\right) \frac{\Omega_{\mathrm{h}}}{\omega_{0}} \Delta u \geq 0,  \tag{4.58}\\
& \Sigma\left(t_{n+1}^{-}\right)=-n \beta_{0, \mathrm{c}} \Delta u+n \beta_{0, \mathrm{~h}} \frac{\Omega_{\mathrm{h}}}{\omega_{0}} \Delta u \geq 0, \tag{4.59}
\end{align*}
$$

at the end of the $n^{\text {th }}$ cycle, where the effective nonequilibrium inverse temperature
$\beta_{\mathrm{h}}^{\star}\left(t_{n}\right)$ of the finite hot bath is computed by solving the equation

$$
\begin{equation*}
n \tanh \left(\frac{\beta_{0, \mathrm{c}} \omega_{0}}{2}\right)+\left(N_{s}-n\right) \tanh \left(\frac{\beta_{0, \mathrm{~h}} \Omega_{\mathrm{h}}}{2}\right)=N_{s} \tanh \left(\frac{\beta_{\mathrm{h}}^{\star}\left(t_{n}\right) \Omega_{\mathrm{h}}}{2}\right) . \tag{4.60}
\end{equation*}
$$

In the left panel of Fig. 4.3, we compare the entropy production $\Sigma$ (4.58) and $\Sigma^{\prime}(4.59)$ as a function of the cycle $n$, which shows that $\Sigma\left(t_{n}\right) \geq \Sigma^{\prime}\left(t_{n}\right)$ at all times consistently with the relation (4.36). In the right panel of Fig. 4.3 we compare the corresponding efficiencies which, accordingly, show that $\eta\left(t_{n}\right) \geq \eta^{\prime}\left(t_{n}\right)$ at all times.

### 4.6 Chapter's outlook

In this chapter we have explored the thermodynamic consequences of the coarsegrained description given by the EMME. In such description, the first law follows from the conservation of the average coarse-grained energy that we discussed in the previous chapter. The second law, requires defining entropy microscopically, and we use the observational entropy to do it. Then, we obtain that during a transformation, the observational entropy always increases, which is our statement of the second law.

In phenomenological thermodynamics, Clausius' inequality quantifies the entropy production that a closed system composed by a "small" open system and heat bath composite experiences after a transformation. Importantly, Clausius' inequality is a consequence of the second law particularized to the aforementioned system-bath composite. In our setup, we found Clausius' inequality as a result of defining the effective nonequilibrium temperature $\beta^{\star}(t)$ that is in one to one correspondence with the average energy of the bath. That is, instead of keeping track of all the bath energy distribution, as the EMME does, Clausius' inequality is only concerned about the bath average energy. For a bath with an infinite heat capacity, one can even replace the effective nonequilibrium temperature $\beta^{\star}(t)$ by the original temperature $\beta_{0}$, which gives rise to yet another level of description that only keeps track of the initial temperature. This forms a hierarchy of second laws that lines up with the hierarchy of master equations that we encountered in the previous chapter.

To conclude, we have explored the use of different second laws to quantify the entropy production and efficiency of a quantum heat engine that operates between a finite and an infinite bath. The use of Clausius' inequality for a finite bath, reveals a universal efficiency improvement as compared to Clausius inequality in the infinite heat capacity limit. We could see this for a particular model that combines the idea of the SWAP engine with the framework of repeated interactions.

In the next chapter, we move beyond weak-coupling master equations and study the dynamics of open quantum systems using the framework of quantum operations. In particular, we explore the spectral properties of general quantum evolutions.

## Spectral properties of quantum evolutions

It is now time to move forward from quantum master equations, and study other approaches to the dynamics of open quantum systems. In this chapter, we introduce the framework of quantum operations to characterize the spectral properties of a quantum evolution. In particular, we start studying the spectral properties of classical stochastic matrices, which correspond to the "population block" of quantum evolutions and that take the form of classical master equations.

Then, we move to the quantum counterpart of the problem. As we have seen in Ch. 2, any quantum map admits a matrix representation in a doubled Hilbert space. This matrix representation encodes some important features of the dynamics in its eigenvalues and eigenvectors. Here, we want to exploit such spectral properties to obtain information about a general quantum dynamics that we denote $\mathcal{E}(t)$. Sometimes, one can proceed further by restricting to the subset of quantum dynamical semigroups, for which $\mathcal{E}(t)=\exp (\mathcal{L} t)$, and study the spectral properties of $\mathcal{L}$. We explore also this route below. Importantly, this chapter is not meant to give a review from all known results in the literature about properties of quantum evolutions. It is rather devoted to review some properties of quantum evolutions, which are of our interest.

Finally, we give two applications, based on the references [RMS20] and [LGR+21],
where the eigenstructure of the quantum evolution is used to provide physical insight about two particular problems.

### 5.1 Warm up: classical stochastic maps

A quantum evolution $\mathcal{E}(t)$ propagates forward in time a certain quantum state $\rho(0)$ as $\rho(t)=\mathcal{E}(t)[\rho(0)]$, while being CPTP. Roughly speaking, these two conditions follow from the requirement that if the input $\rho(0)$ is a quantum state, the output $\rho(t)$ must be also a quantum state.

The classical analog of a quantum evolution is a matrix $E(t)$, which propagates forward in time a certain probability vector $\mathbf{p}(0)$, of components $[\mathbf{p}(0)]_{i}$ $i=1, \cdots, d$, as $\mathbf{p}(t)=E(t) \mathbf{p}(0)$. In terms of components, we can write that $[\mathbf{p}(t)]_{i}=$ $\sum_{j}[E(t)]_{i j}[\mathbf{p}(0)]_{j}$. Similarly to the quantum case, requiring that $\mathbf{p}(t)$ is a probability vector imposes some restrictions on the evolution matrix $E(t)$. Namely,
(a) $[E(t)]_{i j} \geq 0$ for all $i, j=1, \cdots, d$,
(b) $\sum_{i}[E(t)]_{i j}=1$ for all $j=1, \cdots, d$,
where (a) ensures that $\left\{[\mathbf{p}(t)]_{i}\right\}$ is a set of positive numbers, while (b) ensures that add to one $\sum_{i}[\mathbf{p}(t)]_{i}=1$. Conditions (a) and (b) define a stochastic matrix. Some stochastic matrices fulfill a third condition
(c) $\sum_{j}[E(t)]_{i j}=1$ for all $i=1, \cdots, d$.

If a stochastic matrix $E(t)$ fulfills the property (c), then $E(t)$ is known as a bistochastic matrix. Given a bistochastic matrix $E(t)$, the process described by its transpose $E(t)^{T}$ is also a valid classical evolution.

Finally, some classical evolutions $E(t)$ fulfill the semigroup property
(d) $E\left(t+t^{\prime}\right)=E(t) E\left(t^{\prime}\right)$ for all $t, t^{\prime} \in \mathbb{R}$.

If property (d) holds, it is possible to recast the evolution equation of the probability vector $\mathbf{p}$ as equation

$$
\begin{equation*}
\mathbf{p}(t+d t)=E(t+d t) \mathbf{p}(0)=E(d t) \mathbf{p}(t) \approx\left(1_{d}+d t \Lambda\right) \mathbf{p}(t), \tag{5.1}
\end{equation*}
$$

where $\Lambda=\left[\partial_{t} E(t)\right]_{t=0}$ is the generator of the evolution. This leads to the differential equation form

$$
\begin{equation*}
\partial_{t} \mathbf{p}(t)=\Lambda \mathbf{p}(t), \tag{5.2}
\end{equation*}
$$

with solution $E(t)=\exp (\Lambda t)$, which we have encountered several times. Importantly, the properties of $E(t)$ are inherited by $\Lambda$ in the form
(e) $\Lambda_{i j} \geq 0$ for $i \neq j$,
(f) $\sum_{i} \Lambda_{i j}=0$ for $j=1, \cdots, d$,
and if moreover the condition (c) holds we also have
(g) $\sum_{j} \Lambda_{i j}=0$ for $i=1, \cdots, d$.

### 5.1.1 Spectral properties of classical evolutions

Consider a general matrix $Z$. Our aim is to understand which are the vectors $\mathbf{r}$ that are not rotated by the action of $Z$; that is,

$$
\begin{equation*}
Z \mathbf{r}_{i}=z_{i} \mathbf{r}_{i} \tag{5.3}
\end{equation*}
$$

where $z \in \mathbb{C}$ is a scalar. If $\operatorname{det}\left[Z-z 1_{d}\right] \neq 0$, Eq. (5.3) has a unique solution which is trivial $\mathbf{r}=0$. Then, non-trivial solutions $\mathbf{r} \neq 0$ are only possible if $\operatorname{det}\left(Z-z 1_{d}\right)=0$. We define the characteristic polynomial

$$
\begin{equation*}
P_{Z}(z)=\operatorname{det}\left(Z-z 1_{d}\right), \tag{5.4}
\end{equation*}
$$

whose roots $z_{i}$ with $i=1, \cdots, d$ are the eigenvalues of the stochastic matrix $Z$. We order the collection of eigenvalues $\left\{z_{i}\right\}$ is, also known as the spectrum, according to $\left|z_{1}\right| \geq\left|z_{2}\right| \geq \cdots \geq\left|z_{N}\right|$. The non-trivial vectors $\mathbf{r}_{i}$ that solve Eq. (5.3) are the corresponding (right) eigenvectors. For every different, $z_{i}$ there exists at least one eigenvector $\mathbf{r}_{i}$. In the case of eigenvector multiplicity, $z_{i}=z_{j}$, the existence of two (ordinary) eigenvectors $\mathbf{r}_{i} \neq \mathbf{r}_{j}$ is not guaranteed.

Now we assume that $Z$ is a stochastic matrix, that is, it fulfills properties (a) and (b) above. Then the spectrum of $Z$ fulfills
(i) The spectrum of $Z$ belongs to the unit disk $\left|z_{i}\right| \leq 1$, and the leading eigenvalue equals unity $z_{i}=1$.
(ii) The eigenspace associated with $z_{1}$ contains at least a positive eigenstate $\mathbf{p}^{\text {st }} \geq 0$ which is stationary; that is, $Z \mathbf{r}_{1}=\mathbf{r}_{1}$.

The proof of (i) is as follows. First, we note that the characteristic polynomial of a matrix $Z$ is equal to the characteristic polynomial of its transpose $Z^{T}$, which implies that $Z$ and $Z^{T}$ have the same spectrum. Then, we note that using property (b) the eigenvector $(1, \cdots, 1)$ is an eigenvector of $Z^{T}$ with eigenvalue $z=1$, which implies that $Z$ has also an eigenvalue $z=1$. Second, we have to prove that $z=1$
has the largest magnitude. To this end, we introduce the norm $\|\mathbf{r}\|_{1}=\sum_{i}\left|\mathbf{r}_{i}\right|$, and note that

$$
\begin{equation*}
\left|z_{i}\right|\left\|\mathbf{r}_{i}\right\|_{1}=\left\|Z \mathbf{r}_{i}\right\|_{1}=\sum_{j}\left|\sum_{k} Z_{j k}\left(\mathbf{r}_{i}\right)_{k}\right| \leq \sum_{j k} Z_{j k}\left|\left(\mathbf{r}_{i}\right)_{k}\right|=\left\|\mathbf{r}_{i}\right\|_{1}, \tag{5.5}
\end{equation*}
$$

which implies $\left|z_{i}\right| \leq 1$ and $z_{1}=1$. The property (ii) follows by applying (5.5) to $\mathbf{r}_{1}$. We obtain

$$
\begin{equation*}
\left\|\mathbf{r}_{1}\right\|_{1}=\sum_{i}\left|\sum_{j} Z_{i j}\left(\mathbf{r}_{1}\right)_{j}\right| \leq \sum_{i j} Z_{i j}\left|\left(\mathbf{r}_{1}\right)_{j}\right|=\left\|\mathbf{r}_{1}\right\|_{1}, \tag{5.6}
\end{equation*}
$$

and, therefore, the inequality must be saturated, implying that all summands inside the absolute value have the same phase, which we take to be $\left(\mathbf{r}_{1}\right)_{i} \geq 0$. Then, all $\left(\mathbf{r}_{1}\right)_{j}$ are positive and $\mathbf{p}^{\text {st }}=\mathbf{r}_{1} /\left\|\mathbf{r}_{1}\right\|_{1}$ is a stationary probability distribution.

If, moreover, $Z$ is bistochastic; that is, it fulfills property (c), then
(iii) the maximally mixed state $\mathbf{p}^{\text {st }}=(1 / d, \cdots, 1 / d)$ is stationary.
which can be checked by direct computation.

### 5.1.2 Spectral properties of the generator

Having understood the spectrum of a general stochastic matrix $Z=E(t)$, we now investigate the case in which $E(t)$ fulfills property (d); that is, we can rewrite $E(t)=\exp (\Lambda t)$. In particular, we are interested in the spectral properties of the generator $\Lambda$. We start with the property

$$
\begin{equation*}
\Lambda=\lim _{d t \rightarrow 0^{+}} \dot{E}(d t)=\lim _{d t \rightarrow 0^{+}} \frac{E(d t)-1_{d}}{d t} \tag{5.7}
\end{equation*}
$$

which implies that the spectral properties of $\Lambda$ are tightly bounded to the properties of the stochastic matrix $E(d t)$. We note that the eigenvectors of $E(t)$ remain constant, while its eigenvalues depend on time. In particular, given that we know $z_{i}(t)$ and $\mathbf{r}_{i}$ for $Z=E(d t)$, we find

$$
\begin{equation*}
\Lambda \mathbf{r}_{i}=\left[\lim _{d t \rightarrow 0^{+}} \frac{z_{i}(d t)-1}{d t}\right] \mathbf{r}_{i}=: \lambda_{i} \mathbf{r}_{i} . \tag{5.8}
\end{equation*}
$$

and therefore $\Lambda$ and $E(d t)$ share the same (constant) eigenvectors. Clearly, the eigenvalue $z_{1}=1$ of $\mathbf{r}_{1}$ does not depend on time and, therefore, $\Lambda$ has a corresponding eigenvalue $\lambda_{1}=0$. The evolution equation of $\mathbf{p}^{\text {st }}=\mathbf{r}_{1} /\left\|\mathbf{r}_{1}\right\|$ yields $\partial_{t} \mathbf{p}^{\text {st }}=\Lambda \mathbf{p}^{\text {st }}=0$
which, as expected, is a stationary state. Moreover, from Eq. (5.8) and $\left|z_{i}\right| \leq 1$ it is easy to see that $\operatorname{Re} \lambda_{i} \leq 0$; that is, all the eigenvalues $\lambda_{i}$ lie in the non-positive real part of the complex plane.

We have seen that spectral properties of classical stochastic matrices reveal many features of the evolution. Also, those classical stochastic dynamics can appear in certain regimes of the quantum evolution, as it is the case of the energy populations of the BMS master equation. We are now ready to investigate the corresponding properties for a quantum evolution $\mathcal{E}(t)$.

### 5.2 The quantum evolution

We now turn to quantum evolution maps. Consider a Hilbert space $\mathcal{H}$ with a canonical basis $\{|i\rangle\}$ where $i=1, \cdots, d$. Then, a quantum evolution $\mathcal{E}(t)$ evolves a quantum state $\rho(0)$ as $\rho(t)=\mathcal{E}(t)[\rho(0)]$. Requiring that the state $\rho(t)$ remains a valid state for all times $t$ implies that the quantum evolution fulfills the properties
(a') $\mathcal{E}(t)$ is completely positive; that is, $(\mathcal{I} \otimes \mathcal{E}(t))[\circ] \geq 0$ if $\circ \geq 0$, where the identity $\mathcal{I}$ acts on an arbitrary ancillary space,
(b') $\mathcal{E}(t)$ is trace preserving; that is, $\operatorname{tr}\left\{\mathcal{E}(t)\left[{ }^{\circ}\right]\right\}=\operatorname{tr}(\circ)$.
As we encountered in Sec. 2.1.5, properties ( $\mathrm{a}^{\prime}$ ) and ( $\mathrm{b}^{\prime}$ ) holding simultaneously are equivalent to requiring $\mathcal{E}(t)$ to have a Kraus decomposition; that is, $\mathcal{E}(t)[\circ]=$ $\sum_{k} K_{k}(t) \circ K_{k}(t)^{\dagger}$ with $\sum_{k} K_{k}(t)^{\dagger} K_{k}(t)=1_{d}$.

To discuss the spectrum of a CPTP map, we need first to find a matrix representation of it. This can be achieved by the process of "vectorization" that we discussed in Sec. 2.1.5. Namely,

$$
\begin{equation*}
\mathcal{E}(t)=\sum_{i j} \sum_{i^{\prime} j^{\prime}}[\mathcal{E}(t)]_{i j, i^{\prime} j^{\prime} \mid}\left|i j \times i^{\prime} j^{\prime}\right|=\sum_{k} K_{k}(t) \otimes K_{k}(t)^{\star}, \tag{5.9}
\end{equation*}
$$

where the matrix elements $[\mathcal{E}(t)]_{i j, i^{\prime} j^{\prime}}$ correspond to $\langle i| \mathcal{E}(t)\left[\left|i^{\prime} X j^{\prime}\right|\right]|j\rangle$. The vectorized form of a quantum evolution $\mathcal{E}(t)$ is also known as the dynamical matrix.

In this vectorized representation, states $\rho$ becomes vectors $|\rho\rangle\rangle$ and the inner product $\langle\langle\sigma \mid \rho\rangle\rangle=\operatorname{tr}\left[\sigma^{\dagger} \rho\right]$ corresponds to the Hilbert-Schmidt product. An important notion is that of the dual of a quantum map with respect to the Hilbert-Schmidt product. Namely, the dual map $\mathcal{E}(t)^{\ddagger}$ is defined as the one that fulfills

$$
\begin{equation*}
\langle\langle\sigma \mid \mathcal{E}(t)[\rho]\rangle\rangle=\operatorname{tr}\left[\sigma^{\dagger} \mathcal{E}(t)[\rho]\right]=\operatorname{tr}\left[\left(\mathcal{E}(t)^{\ddagger}[\sigma]\right)^{\dagger} \rho\right]=\left\langle\left\langle\mathcal{E}(t)^{\ddagger}[\sigma] \mid \rho\right\rangle\right\rangle, \tag{5.10}
\end{equation*}
$$

for any pair of elements $\rho, \sigma \in \operatorname{Op}(\mathcal{H})$. The dual map can be interpreted as the quantum evolution in the Heisenberg picture. Moreover, its explicit expression can be found in terms of the Kraus operators to be $\mathcal{E}(t)^{\ddagger}\left[{ }^{\circ}\right]=\sum_{k} K_{k}(t)^{\dagger} \circ K_{k}(t)$. Therefore, it is a completely positive and identity preserving map since $\mathcal{E}(t)^{\ddagger}\left[\mathbf{1}_{d}\right]=$ $\mathbf{1}_{d}$. Trace preservation and unit preservation are dual properties: the dual of a trace-preserving map preserves the identity and vice versa. This property will be crucial in the following.

Some CPTP maps are also identity preserving and fulfill the third condition
(c') $\mathcal{E}(t)\left[\mathbf{1}_{d}\right]=\mathbf{1}_{d}$,
which implies that the dual map $\mathcal{E}(t)^{\ddagger}$ is also a valid quantum evolution.
Finally, some maps also fulfill the semigroup property
(d') $\mathcal{E}\left(t+t^{\prime}\right)=\mathcal{E}(t) \mathcal{E}\left(t^{\prime}\right)$ for all $t, t^{\prime} \in \mathbb{R}$.
If property ( $d^{\prime}$ ) holds, it is possible to recast the evolution equation of a state $\rho(t)$ as

$$
\begin{equation*}
\rho(t+d t)=\mathcal{E}(t+d t) \rho(0)=\mathcal{E}(d t) \rho(t) \approx(\mathcal{I}+d t \mathcal{L}) \rho(t) \tag{5.11}
\end{equation*}
$$

where $\mathcal{L}=\left[\partial_{t} \mathcal{E}(t)\right]_{t=0}$ is the generator of the evolution. This leads to a differential equation of the form of a quantum master equation

$$
\begin{equation*}
\partial_{t} \rho=\mathcal{L}[\rho(t)], \tag{5.12}
\end{equation*}
$$

with the solution $\mathcal{E}(t)=\exp (\mathcal{L} t)$, as it was the case for the BMS master equation. Again, the properties of $\mathcal{E}(t)$ are inherited by $\mathcal{L}$ in the form
(e') $\mathcal{L}$ is of the Gorini-Kossakowski-Sudarshan-Lindblad form,
(f') $\mathcal{L}$ is traceless in the sense that $\operatorname{tr}\{\mathcal{L}[\circ]\}=0$,
and if moreover ( $\mathrm{c}^{\prime}$ ) holds also
(g') $\mathcal{L}^{\ddagger}$ is traceless in the sense that $\operatorname{tr}\left\{\mathcal{L}^{\ddagger}[0]\right\}=0$.
Properties (a')-(g') are the analogous to the properties (a)-(g) and, for this reason, quantum evolutions are taken to be the quantum counterpart of the classical stochastic matrices. In the following, we see that this analogy also determines similar spectral properties for classical and quantum stochastic maps.

### 5.3 Spectral properties of the quantum evolution

Consider a general quantum map $\mathcal{Z}$. As before, our aim is to understand which right vectorized operators $\left|R_{\mu}\right\rangle$ are not "rotated" by the action of the dynamical matrix $\mathcal{Z}$. That is,

$$
\begin{equation*}
\left.\left.\mathcal{Z}\left[R_{\mu}\right]=z_{\mu} R_{\mu} \Leftrightarrow \mathcal{Z}\left|R_{\mu}\right\rangle\right\rangle=z_{\mu}\left|R_{\mu}\right\rangle\right\rangle, \tag{5.13}
\end{equation*}
$$

where $z_{\mu} \in \mathbb{C}$. This is only possible for the $d^{2}$ roots of the characteristic polynomial $P_{\mathcal{Z}}(z)=\operatorname{det}\left(\mathcal{Z}-z 1_{d^{2}}\right)$. Again, we order the eigenvalues according to $\left|z_{1}\right| \geq\left|z_{2}\right| \geq$ $\cdots \geq\left|z_{d^{2}}\right|$. For every different $z_{\mu}$, there is at least one non-trivial eigenmatrix $R_{\mu}$ that fulfills Eq. (5.13). Similarly, we can consider the left eigenvalue equation

$$
\begin{equation*}
\left.\left.\mathcal{Z}^{\ddagger}\left|L_{\mu}\right\rangle\right\rangle=z_{\mu}\left|L_{\mu}\right\rangle\right\rangle \Leftrightarrow\left\langle\left\langle L_{\mu}\right| \mathcal{Z}=z_{\mu}\left\langle\left\langle L_{\mu}\right|,\right.\right. \tag{5.14}
\end{equation*}
$$

which shares the same spectrum $\left\{z_{\mu}\right\}$.
Assuming that $\mathcal{Z}$ is a CPTP map; that is, it fulfills properties (a') and (b') above, we find that
(i') The spectrum of $\mathcal{Z}$ belongs to the unit disk $\left|z_{\mu}\right| \leq 1$, and the leading eigenvalue equals unity $z_{\mu}=1$.
(ii') The eigenspace associated with $z_{1}$ contains at least a positive eigenstate $\rho^{\text {st }} \geq 0$ which is stationary; that is, $\mathcal{Z}\left[\rho^{\text {st }}\right]=\rho^{\text {st }}$.

As it turns out, it is easier to argue about the spectrum of the dual map $\mathcal{Z}^{\ddagger}$, which is identity preserving and has the same spectrum as $\mathcal{Z}$. We proceed as follows.

Let $L_{\mu}$ be a left eigenvector of $\mathcal{Z}$ with eigenvalue $z_{\mu}$ an

$$
A:=\left(\begin{array}{cc}
\mathbf{1}_{d} & L_{\mu}  \tag{5.15}\\
L_{\mu}^{\dagger} & \alpha \mathbf{1}_{d}
\end{array}\right),
$$

be a matrix in the extended space $\mathbb{C}^{2} \otimes \mathcal{H}$, where $\alpha \geq 0$ is the largest eigenvalue of the positive operator $L_{\mu}^{\dagger} L_{\mu}$. The Schur complement $S_{\mathrm{c}}[A]$ of the matrix $A$ yields

$$
\begin{equation*}
S_{\mathrm{c}}[A]:=\alpha \mathbf{1}_{d}-L_{\mu}^{\dagger} L_{\mu} \geq 0, \tag{5.16}
\end{equation*}
$$

which, with our choice of $\alpha$, is positive semidefinite. By completeness, we show in App. C. 1 that the Schur complement of a matrix is positive if and only if the matrix
is positive; that is, $S_{\mathrm{c}}[A] \geq 0 \Leftrightarrow A \geq 0$. Using the completely positive and identity preserving properties we see that if $A \geq 0$ also the matrix

$$
A^{\prime}:=\left(\mathcal{I}_{2} \otimes \mathcal{Z}^{\ddagger}\right)[A]=\left(\begin{array}{cc}
\mathbf{1}_{d} & \mathcal{Z}^{\ddagger}\left[L_{\mu}\right]  \tag{5.17}\\
\left\{\mathcal{Z}^{\ddagger}\left[L_{\mu}\right]\right\}^{\dagger} & \alpha \mathbf{1}_{d}
\end{array}\right) \geq 0,
$$

is positive. Hence, the Schur complement of $A^{\prime}$ has to be positive, which implies that

$$
\begin{equation*}
S_{\mathrm{c}}\left[A^{\prime}\right]:=\alpha \mathbf{1}_{d}-\left\{\mathcal{Z}^{\ddagger}\left[L_{\mu}\right]\right\}^{\dagger} \mathcal{Z}^{\ddagger}\left[L_{\mu}\right]=\alpha \mathbf{1}_{d}-\left|z_{\mu}\right|^{2} L_{\mu}^{\dagger} L_{\mu} \geq 0 \tag{5.18}
\end{equation*}
$$

Subtracting Eq. (5.16) from Eq. (5.18), we arrive at the condition $\left|z_{\mu}\right| \leq 1$; that is, the spectrum lies in the unit disk. Also, the identity preserving property of $\mathcal{Z}^{\ddagger}$ which implies that $L_{1}=\mathbf{1}_{d}$ has the eigenvalue $z_{1}=1$, which concludes the proof of (i').

To prove (ii'), we use that completely positive maps also fulfill that $\mathcal{Z}\left[{ }^{\dagger}{ }^{\dagger}\right]=\mathcal{Z}\left[0^{\dagger}\right]^{\dagger}$, which can be easily checked from the Kraus decomposition. This implies that if $R_{\mu}$ is an eigenmatrix with eigenvalue $z_{\mu}$, then $R_{\mu}^{\dagger}$ is also an eigenmatrix with eigenvalue $z_{\mu}^{*}$. In other words, complex eigenvalues come in pairs $\left\{z_{\mu}, z_{\mu}^{*}\right\}$. This property implies that eigenmatrices of real eigenvalue $z_{\mu}^{*}$ can be chosen to be Hermitian; that is, if $R_{\mu}$ is an eigenmatrix with real eigenvalue, the combinations $\left(R_{\mu}+R_{\mu}^{\dagger}\right) / 2$ and $\left(R_{\mu}-R_{\mu}^{\dagger}\right) /(2 i)$ are Hermitian eigenmatrices with the same eigenvalue. In turn, this implies that $R_{1}$ can be diagonalized and has real eigenvalues. Hence, it admits the decomposition $R_{1}=R_{1,+}-R_{1,-}$, where $R_{1, \pm} \geq 0$. Let $P_{ \pm}$denote the projectors onto the positive and negative subspaces; that is, $P_{ \pm} R_{1}=R_{1, \pm}$.

$$
\begin{equation*}
\operatorname{tr}\left(R_{1,+}\right)=\operatorname{tr}\left\{P_{+} \mathcal{Z}\left[R_{1,+}\right]+P_{+} \mathcal{Z}\left[R_{1,-}\right]\right\} \leq \operatorname{tr}\left\{P_{+} \mathcal{Z}\left(R_{1,+}\right)\right\} \leq \operatorname{tr}\left\{\mathcal{Z}\left[R_{+}\right]\right\}=\operatorname{tr}\left(R_{1,+}\right), \tag{5.19}
\end{equation*}
$$

then, the two inequalities must be equalities. The first inequality implies that $P_{+} \mathcal{Z}\left[R_{1,-}\right]=0$, while the second that $P_{-} \mathcal{Z}\left[R_{1,+}\right]=0$. Hence, $R_{1,+} \geq 0$ is an eigenmatrix with eigenvalue $z_{1}=1$, which concludes the proof of property (ii').

If, moreover, $\mathcal{Z}$ fulfills property ( $c^{\prime}$ ), we also have that
(iii') the maximally mixed state $\rho^{\text {st }}=R_{1}=\mathbf{1}_{d} / d$ is stationary,
which is checked by direct computation.

### 5.3.1 Spectral properties of the Lindbladian

Having understood the spectral properties of completely positive and trace preserving maps, we consider now quantum evolutions that fulfill property (d'). We
are interested in the spectral properties of the generator of that evolution,

$$
\begin{equation*}
\mathcal{L}=\lim _{d t \rightarrow 0^{+}} \mathcal{E}(d t)=\lim _{d t \rightarrow 0^{+}} \frac{\mathcal{E}(d t)-\mathcal{I}}{d t} \tag{5.20}
\end{equation*}
$$

We consider now $\mathcal{Z}=\mathcal{E}(t)$, in such a way that

$$
\begin{equation*}
\mathcal{L} R_{\mu}=\left[\lim _{d t \rightarrow 0^{+}} \frac{z_{\mu}(d t)-1}{d t}\right] R_{\mu}=: \lambda_{\mu} R_{\mu}, \tag{5.21}
\end{equation*}
$$

and, then, $\mathcal{L}$ and $\mathcal{E}(t)$ share the same eigenvectors. Clearly, the eigenvalue $z_{1}=1$ is time-independent and, therefore, $\mathcal{L}$ has a corresponding eigenvalue $\lambda_{1}=0$. Then, the evolution equation of $\rho^{\text {st }}=R_{1} / \operatorname{tr}\left[R_{1}\right] \geq 0$ yields simply $\partial_{t} \rho^{\text {st }}=\mathcal{L}\left[\rho^{\text {st }}\right]=0$ and corresponds to a stationary state. Again, all the eigenvalues $\lambda_{\mu}$ lie in the negative real part half plane, since $\operatorname{Re}\left[z_{\mu}(t)\right] \leq 1$ for all eigenvalues in the unit disk $\left|z_{\mu}(t)\right| \leq 1$. Therefore, all $\operatorname{Re} \lambda_{\mu} \leq 0$ for all $\lambda_{\mu}$.

### 5.3.2 The Jamiołkowski-Choi state

So far, we have taken the "vectorized" version of a CPTP map $\mathcal{Z}$; that is, the dynamical matrix, to be the most natural choice of a matrix representation for the map. As it turns out, such a representation is not unique. Here, we introduce an alternative matrix description of $\mathcal{Z}$ which establishes a connection between quantum maps and quantum states: the Jamiołkowski-Choi state.

Consider $\mathcal{Z}$ that acts on matrices defined in the Hilbert space $\mathcal{H}_{\mathrm{A}}$, with a canonical basis $\{|i\rangle\} i=1, \cdots, d$, and $\mathcal{H}_{\mathrm{B}}$ which is a copy of $\mathcal{H}_{\mathrm{A}}$. We define the state $\left|\Psi_{+}\right\rangle=d^{-1 / 2} \sum_{i^{\prime}}\left|i^{\prime} i^{\prime}\right\rangle \in \mathcal{H}_{B} \otimes \mathcal{H}_{\mathrm{A}}$. Then, the Jamiołkowski-Choi state is defined as

$$
\begin{equation*}
\rho_{\mathcal{Z}}:=(\mathcal{Z} \otimes \mathcal{I})\left[\left|\Psi_{+} X \Psi_{+}\right|\right]=\frac{1}{d} \sum_{i^{\prime} j^{\prime}} \mathcal{Z}\left[\left|i^{\prime} X j^{\prime}\right|\right] \otimes\left|i^{\prime} X j^{\prime}\right|=\frac{1}{d} \sum_{i j i^{\prime} j^{\prime}} \mathcal{Z}_{i j i^{\prime} j^{\prime}}\left|i i^{\prime} X j j^{\prime}\right| . \tag{5.22}
\end{equation*}
$$

Hence, the Jamiołkowski-Choi state $\rho_{\mathcal{Z}}$ contains all the information about the output-input relations of the map in the same way that the vectorized map $\mathcal{Z}$ did. In fact, $\rho_{\mathcal{Z}}$ is just a reshuffled version of the vectorized map $\mathcal{Z}$

$$
\begin{equation*}
\left(\rho_{\mathcal{Z}}\right)_{i i^{\prime} j^{\prime}}=\mathcal{Z}_{i j i^{\prime} j^{\prime}} \tag{5.23}
\end{equation*}
$$

The trace preserving property of $\mathcal{Z}$ is inherited by the Jamiołkowski-Choi state as the property

$$
\begin{equation*}
\operatorname{tr}_{\mathrm{B}}\left[\rho_{z}\right]=\frac{\mathbf{1}_{d}}{d} . \tag{5.24}
\end{equation*}
$$

Moreover, since the map $\mathcal{Z}$ is completely positive, the resulting Jamiołkowski-Choi state is a positive matrix $\rho_{\mathcal{Z}} \geq 0$ and, in particular, Hermitian. On the plus side, this implies that, unlike the vectorized map $\mathcal{Z}, \rho_{\mathcal{Z}}$ is diagonalizable and has positive eigenvalues. On the downside, the corresponding eigenproperties of $\rho_{\mathcal{Z}}$ cannot be straightforwardly interpreted.

In order to give an interpretation to the eigendecomposition of the JamiołkowskiChoi state, we write explicitly the components $\mathcal{Z}_{i j i^{\prime} j^{\prime}}$ in the definition (5.22) using the Kraus operators. This leads to

$$
\begin{equation*}
\left.\rho_{\mathcal{Z}}=\frac{1}{d} \sum_{k}\left(\sum_{i^{\prime} i} K_{k, i i^{\prime}}\left|i i^{\prime}\right\rangle\right)\left(\sum_{j j^{\prime}} K_{k, j j^{\prime}}\left|j j^{\prime}\right\rangle\right)^{\dagger}=\frac{1}{d} \sum_{k}\left|K_{k}\right\rangle\right\rangle\left\langle\left\langle K_{k}\right|,\right. \tag{5.25}
\end{equation*}
$$

where $\left.\left|K_{k}\right\rangle\right\rangle=\sum_{i i^{\prime}} K_{k, i i^{\prime}}\left|i i^{\prime}\right\rangle$ is the vectorized form of the Kraus operators. Equation (5.25) is closely related to the eigendecomposition of $\rho_{\mathcal{Z}}$. The eigenvalues of $\rho_{\mathcal{Z}}$ are $\left\langle\left\langle K_{k} \mid K_{k}\right\rangle\right\rangle / d$, while the normalized eigenvectors correspond to $\left.\left|K_{k}\right\rangle\right\rangle / \sqrt{\left.\left\langle K_{k} \mid K_{k}\right\rangle\right\rangle}$ to the vectorized form of the Kraus operators.

In the following, we consider two applications that make use of the spectral properties of quantum evolutions to study two very different problems of interest. The first, uses the Jamiołkowski-Choi state representation of a quantum channel to obtain the most general form of a CPTP map that achieves a certain task. The second, studies quantum evolutions that form a quantum-semigroup and that admit more than one stationary state.

### 5.4 Application I: spectral properties of open discrete time crystals

Time crystals are a novel phase of matter that was proposed by Frank Wilczek in 2012 [Wil12]. A time crystal is a phase of matter in which the system breaks time translational symmetry. This behavior is analogous to the usual "space crystals" which break the space translational symmetry of the Hamiltonian. As we shall see, the particular properties of discrete time crystals in open quantum systems are reflected in its eigenvalues, which makes the spectral study of the corresponding quantum evolution a promising approach to understand this phase of matter.

The Hamiltonian of a physical system can have a continuous time symmetry $H(t)=H(t+\tau)$ with $\tau \in \mathbb{R}$ ( $H$ is time-independent) or a discrete time symmetry $H(t)=H\left(t+\tau_{\mathrm{d}}\right)$, where $\tau_{\mathrm{d}}$ is the driving period. Time crystals as conceived by Wilczek are not possible in closed quantum systems that have a continuous time
symmetry (see [KMS19] for an enlarged the discussion). Instead, discrete time crystals can break the discrete time symmetry of a periodically driven Hamiltonian, giving rise to a response function $f_{X}(t)=\operatorname{tr}\left[X \rho_{\mathrm{S}}(t)\right]$ associated to an observable $X$, that does not share the periodicity of the Hamiltonian; that is, $f_{X}(t) \neq f_{X}\left(t+\tau_{\mathrm{d}}\right)$. For discrete time crystals, the symmetry is recovered after a certain number of driving periods $M$, such that $f_{X}\left(t+M \tau_{\mathrm{d}}\right)=f_{X}(t)$, which is known as subharmonic response since it has a frequency $2 \pi /\left(M \tau_{\mathrm{d}}\right)$. Typical time crystal phases are engineered to have the so-called period-doubling response, in which $f(t)=f\left(t+2 \tau_{\mathrm{d}}\right) \neq f\left(t+\tau_{\mathrm{d}}\right)$. For instance, period-doubling discrete time crystals are often implemented in condensed matter systems with parity symmetry. The system is prepared in one of the two symmetry broken ground states, and the driving implements a unitary transition that maps one into the other, giving rise to a response with period $2 \tau_{\mathrm{d}}$.

Time crystals are distinguished from other time-periodic oscillations, such as Rabi oscillations, because the frequency of the oscillations is robust to small perturbations. Namely, if the driving protocol is implemented with a certain error, one expects the response to still exhibit the symmetry breaking. Moreover, the oscillations should persist ideally to infinite time.

Experimentally, the observation of time-crystalline behavior in closed quantum systems have been reported [CCL+17; ZHK+17]. In those experiments, dissipation and decoherence were seen as detrimental effects for the time-crystal. Recently, it has been proposed to use the unavoidable dissipation and decoherence to stabilize the time crystal, which has led to the study of time crystallinity in open quantum systems. While a lot of research is missing in this direction, the first steps towards the understanding of this phenomenon have been already taken, resulting in both theoretical [GHU18] and experimental [KKG+21] advances.

### 5.4.1 Quantum evolution and Floquet map of a periodic evolution

Here, we discuss how to translate the properties of discrete time crystal in open systems to the spectral properties of the so-called Floquet map. We start our discussion by considering a general time-periodic system whose evolution equation is given by

$$
\begin{equation*}
\partial_{t} \rho_{\mathrm{S}}=\mathcal{L}(t)\left[\rho_{\mathrm{S}}\right]=\mathcal{L}\left(t+\tau_{\mathrm{d}}\right)\left[\rho_{\mathrm{S}}\right] \tag{5.26}
\end{equation*}
$$

where $\tau_{\mathrm{d}}$ is the driving period. The quantum evolution $\mathcal{E}(t)\left[{ }^{\circ}\right]$ that solves Eq. (5.26) takes the form of a time-ordered exponential, and it is given by

$$
\begin{equation*}
\mathcal{E}(t)=\exp _{+}\left[\int_{0}^{t} d t^{\prime} \mathcal{L}\left(t^{\prime}\right)\right] \tag{5.27}
\end{equation*}
$$

which is a completely positive and trace preserving map. Because the generator of the evolution $\mathcal{E}(t)$ is periodic; that is, $\mathcal{L}(t)=\mathcal{L}\left(t+\tau_{\mathrm{d}}\right)$, the evolution at times $t_{m}=m \tau_{\mathrm{d}}$ with $m \in \mathbb{N}$ can be written as

$$
\begin{equation*}
\rho_{\mathrm{s}}\left(t_{m}\right)=\mathcal{E}\left(\tau_{\mathrm{d}}\right)\left[\rho_{\mathrm{S}}\left(t_{m-1}\right)\right]=\mathcal{E}\left(\tau_{\mathrm{d}}\right)^{m}\left[\rho_{\mathrm{s}}(0)\right]=: \mathcal{Z}^{m}\left[\rho_{\mathrm{s}}(0)\right] . \tag{5.28}
\end{equation*}
$$

where we call $\mathcal{Z}$ the Floquet map, and encodes the information about the evolution of the system at the stroboscopic times $t_{m}$.

There are two important notions associated with the Floquet map $\mathcal{Z}$ that are useful for the subsequent discussion. Consider the eigenvalue equation $\mathcal{Z}\left[R_{\mu}\right]=$ $z_{\mu} R_{\mu}$. The first notion is the asymptotic subspace $\operatorname{As}(\mathcal{Z})$ of the Floquet map $\mathcal{Z}$, that we define as $\operatorname{As}(\mathcal{Z}):=\operatorname{span}\left(R_{\mu}:\left|z_{\mu}\right|=1\right)$. The elements of the asymptotic subspace $\operatorname{As}(\mathcal{Z})$ determine the long-time behavior of the dynamics. The second notion is the dissipative Floquet gap

$$
\begin{equation*}
\Delta:=-\frac{1}{\tau_{\mathrm{d}}} \max _{z_{\mu}:\left|z_{\mu}\right| \neq 1} \log \left|z_{\mu}\right|, \tag{5.29}
\end{equation*}
$$

whose inverse determines the timescale of decay towards the asymptotic subspace.

### 5.4.2 Time crystals as spectral properties of the Floquet map

As discussed in the introduction, time crystals in closed systems are identified by exhibiting: (i) a discrete time-translational symmetry breaking that persists to infinite time and (ii) a robust subharmonic response. Analogously, we define an open quantum system to be in the discrete time crystal phase if its Floquet map satisfies
(i) There exists at least one eigenvalue $z_{\mu}$ such that $z_{\mu} \neq 1$ but $z_{\mu}^{M}=1$ for some integer $M>1$. We denote such eigenvalue by $z_{*}$.
(ii) Given a linear deformation of the Floquet map $\mathcal{Z} \mapsto \mathcal{Z}(\epsilon)=\mathcal{Z}+\epsilon \mathcal{V}$ for a reasonable perturbation $\mathcal{V}$, the eigenvalue $z_{\star}$ is linearly robust; that is, $\left[\partial_{\epsilon} z_{\star}(\epsilon)\right]_{\epsilon=0}=0$.


Figure 5.1: Typical spectrum of the Floquet operator corresponding to the timecrystal phase. The eigenvalues corresponding to the asymptotic space (colored in blue) are $z_{1}=1$ and $z_{2}=z_{\star}=-1$. The decaying states (colored in red) decay with a timescale fixed by the Floquet gap $\Delta$.

In the opposite case, the system becomes periodic with period $\tau_{\mathrm{d}}$ and reaches the trivial phase. In Fig. 5.1 we show the typical spectrum of the Floquet operator corresponding to the time-crystal phase, which has two eigenmatrices in the asymptotic subspace $\mathrm{As}(\mathcal{Z})$.

Some remarks are in order. First, we are assuming that we are able to measure an observable $X$ whose average $f_{X}(t)$ detects the discrete time translation symmetry breaking. In principle, the observable $X$ could have the same average over two different states $\rho\left(t_{m}\right) \neq \rho\left(t_{m+1}\right)$ in such a way that, despite having subharmonic response, $f_{X}(t)$ cannot detect it. Second, we require the subharmonic response to be robust with respect to reasonable perturbations $\mathcal{V}$. The "reasonable" perturbations depend on the particular periodic driving. Typically, $\mathcal{V}$ is considered an error due to disordered rotation errors or global rotation errors (see the following subsection). Finally, our definition of the time crystal phase does not correspond to a "phase of matter" in the usual sense. Simply, a system fulfilling (i) and (ii) displays infinitelylived and robust subharmonic response, which are necessary conditions for a time crystal to exist.


Figure 5.2: Sketch of the time crystalline behavior of the periodically driven XY chain of $N=6$ spins.

### 5.4.3 Example: the open XY model

Let us investigate the stability of an open discrete time crystal in the paradigmatic XY chain, described by the Hamiltonian

$$
\begin{equation*}
H_{S}=-J \sum_{r=1}^{N}\left(\frac{1+g}{2} \sigma_{r}^{x} \sigma_{r+1}^{x}+\frac{1-g}{2} \sigma_{r}^{y} \sigma_{r+1}^{y}+h \sigma_{r}^{z}\right) \tag{5.30}
\end{equation*}
$$

which represents a one dimensional chain of $N$ spins that interact anisotropically. In Eq. (5.30), $J$ is an energy scale, $g$ is the anisotropy constant, and $h$ is the dimensionless transverse field. We consider periodic boundary conditions in such a way that $\sigma_{r}^{x, y, z}=\sigma_{N+r}^{x, y, z}$ and, for technical reasons, we restrict ourselves to an even number of sites $N$. A sketch of this model is shown in Fig. 5.2.

This model and its symmetries have been largely investigated in the literature, for instance, see [Fra17]. For our purposes, it is sufficient to mention that the Hamiltonian $H_{\mathrm{S}}$ in Eq. (5.30) is symmetric under the parity operator $P=\prod_{r=1}^{N} \sigma_{r}^{z}$; that is $P H_{\mathrm{S}} P=H_{\mathrm{s}}$. This implies that $H_{\mathrm{S}}$ can be block-diagonalized into blocks of fixed parity value $p= \pm 1$. We use the notation $|\mathrm{GS}, p\rangle$ to denote the corresponding ground state of each parity block.

We consider the XY chain to be in weak contact with a bosonic heat bath. Namely, the total Hamiltonian takes is of the form $H=H_{\mathrm{S}}+H_{\text {int }}+H_{\mathrm{B}}$, where the
interaction Hamiltonian is taken of the form

$$
\begin{equation*}
H_{\mathrm{int}}=\lambda M_{z} \otimes B:=\lambda \sum_{k} \sum_{r=1}^{N} c_{k} \sigma_{r}^{z} \otimes\left(b_{k}^{\dagger}+b_{k}\right), \tag{5.31}
\end{equation*}
$$

where $M_{z}=\sum_{r=1}^{N} \sigma_{r}^{z}$ is the magnetization along the z-axis, and

$$
\begin{equation*}
H_{\mathrm{B}}=\Omega_{k}\left(b_{k}^{\dagger} b_{k}+\mathbf{1} / 2\right) \tag{5.32}
\end{equation*}
$$

With the interaction (5.31), the parity $P$ becomes a strong symmetry of the dynamics since $[P, H]=0$. Also, we note that the coupling to the bath is global in the sense that all particles are identically coupled to the reservoir bosonic mode $k$ of the heat bath. Then, combining the results of Sec. 2.2.3 and Sec. 2.4.1 we find a weak-coupling master equation for the reduced state of the system that yields $\partial_{t} \rho_{\mathrm{S}}(t)=\mathcal{L}\left[\rho_{\mathrm{S}}\right]$, where $\mathcal{L}$ is of the form of the BMS generator. At zero temperature, when the heat bath is found has $\beta \rightarrow \infty$, the dissipation brings the system closer to the ground subspace. The quantum evolution $\mathcal{E}(t)$ can be seen to have more than one eigenvalue with modulus one. For instance, any matrix element of the form $\left|\mathrm{GS}, p \times \mathrm{GS}, p^{\prime}\right|$ with $p, p^{\prime}= \pm 1$ is stationary.

The final part for our model is the periodic driving. We assume that the XY chain is "kicked" periodically with the Hamiltonian

$$
\begin{equation*}
H_{\mathrm{K}}(t)=\frac{k_{0}}{2} \sum_{m=1}^{\infty} M_{z} \delta\left(t-m \tau_{\mathrm{d}}\right), \tag{5.33}
\end{equation*}
$$

where $k_{0}$ is the kick strength, at regular times $t_{m}=m \tau_{\mathrm{d}}$ with $m=1,2, \cdots$. The unitary transformation $U_{\mathrm{K}}$ induced in the system after one of the pulses has interacted with it is

$$
\begin{equation*}
U_{K}=\exp \left(-i k_{0} \sum_{r=1}^{N} \sigma_{r}^{z}\right)=\prod_{r=1}^{N}\left(\cos \left(k_{0} / 2\right) \mathbf{1}_{2}-i \sin \left(k_{0} / 2\right) \sigma_{r}^{z}\right) . \tag{5.34}
\end{equation*}
$$

For instance, for $k_{0}=\pi$ the unitary transformation $U_{K}$ equals to the parity operator $P$ up to an unimportant phase. The corresponding Floquet map is computed in its vectorized form as

$$
\begin{equation*}
\mathcal{Z}=U_{\mathrm{K}} \otimes U_{\mathrm{K}}^{*} \exp \left(\mathcal{L} \tau_{\mathrm{d}}\right) \tag{5.35}
\end{equation*}
$$

Then, in order to implement the discrete time crystal in the XY spin chain, we consider the following protocol. First, the system is prepared in the superposition state

$$
\begin{equation*}
\rho(0)=\frac{1}{2}(|\mathrm{GS},+\rangle+|\mathrm{GS},-\rangle)(\langle\mathrm{GS},+|+\langle\mathrm{GS},-|), \tag{5.36}
\end{equation*}
$$

which is invariant under the dissipative dynamics $\exp \left(\mathcal{L} \tau_{\mathrm{d}}\right)$. Then, if we kick the system with strength $k_{0}=\pi$, and repeat the operation for $m$ driving periods, we obtain

$$
\begin{equation*}
\rho\left(t_{m}\right)=\frac{1}{2}\left(|\mathrm{GS},+\rangle+(-)^{m}|\mathrm{GS},-\rangle\right)\left(\langle\mathrm{GS},+|+(-)^{m}\langle\mathrm{GS},-|\right), \tag{5.37}
\end{equation*}
$$

which displays subharmonic oscillations. We note that the magnetization per spin along the x-axis $m_{x}:=N^{-1} \sum_{r=1}^{N} \sigma_{r}^{x}$ transforms under the parity as

$$
\begin{equation*}
P m_{x} P=-m_{x} . \tag{5.38}
\end{equation*}
$$

The same effect happens for the magnetization along the $y$-axis. Hence, the corresponding response function

$$
\begin{equation*}
f_{m_{x}}\left(t_{m}\right)=(-)^{m} f_{m_{x}}(0) \tag{5.39}
\end{equation*}
$$

displays subharmonic oscillations that last, ideally, up to infinite time.
Finally, it is left to check whether the subharmonic oscillations are robust. We consider two types of perturbations in our protocol: (a) a disordered rotation error and (b) a global rotation error.

The disordered rotation error (a) is induced by a kick Hamiltonian with a site dependent disorder

$$
\begin{equation*}
H_{\mathrm{K}}(t)=\sum_{m} \delta\left(t-m \tau_{\mathrm{d}}\right) \sum_{r=1}^{N}\left(\pi+\epsilon \delta_{r}\right) \frac{\sigma_{r}^{z}}{2}, \tag{5.40}
\end{equation*}
$$

where the small parameter $\epsilon$ parametrizes the disorder strength, and $\delta_{r}$ measures is the fluctuation at site $r$, which is subject to $\sum_{r} \delta_{r}=0$. To first order in $\epsilon$, the corresponding perturbation $\mathcal{V}_{\text {dis }}$ is

$$
\begin{equation*}
\mathcal{V}_{\mathrm{dis}}(\circ)=-i \frac{1}{2} \sum_{r} \delta_{r}\left[\sigma_{r}^{z}, \mathcal{Z}(\circ)\right] . \tag{5.41}
\end{equation*}
$$

The linear correction of the perturbed eigenvalues $z_{\mu}(\epsilon)$ of the perturbed Floquet map $\mathcal{Z}(\epsilon)=\mathcal{Z}+\epsilon \mathcal{V}_{\text {dis }}$ can be computed using perturbation theory (see App. C.2)

$$
\begin{equation*}
\left[\partial_{\epsilon} z_{\mu}(\epsilon)\right]_{\epsilon=0}=-\frac{i}{2} \sum_{r} \delta_{r} \operatorname{tr}\left\{L_{\mu}^{\dagger}\left[\sigma_{r}^{z}, \mathcal{Z}\left(R_{\mu}\right)\right]\right\}=z_{\mu} \frac{i}{2}\left(\sum_{r} \delta_{r}\right) \operatorname{tr}\left\{L_{\mu}\left[\sigma_{1}^{z}, R_{\mu}\right]\right\} \tag{5.42}
\end{equation*}
$$

where we have used the permutationally invariance of the system. Therefore, the time crystal is linearly robust to a disordered rotation error.


Figure 5.3: Subharmonic oscillations in the open XY time crystal for three global error values $\epsilon=0$ (orange line with circle markers), $\epsilon=\pi / 20$ (blue line with triangular markers), and (yellow line with diamond markers) for a chain of $N=6$ spins. (left panel) Robust subharmonic oscillations of the response function $f_{X}(t)$ with $X=m_{x}$ the magnetization per spin along the x -axis. (right panel) Less robust subharmonic oscillations of the response function $f_{X}(t)$ for $X=\sin (\varphi) m_{x}+\cos (\varphi) m_{y}$ where the angle $\varphi$ fulfills $\cos (\varphi)=\sqrt{(1+g) /(1-g)}$. Parameters are $\tau_{\mathrm{d}}=100 / \mathrm{J}$, $\beta=\infty, J(\omega)=\gamma_{0} \omega, \gamma_{0}=0.01 \mathrm{~J}$.

For the global rotation error type of perturbation (b), we have to rely on numerics. In Fig. 5.3, we show the subharmonic oscillations for chain of $N=6$ spins with parameters $g=1$ and $h=0$ (left panel) and $g=1 / \sqrt{2}$ and $h=1 / \sqrt{2}$ (right panel). For each parameter set, we consider rotation errors $\epsilon=(0, \pi / 40, \pi / 20)$. As the initial state of the evolution we take $\rho(0)$ in Eq. (5.36). In the left panel of Fig. 5.3 we observe that the oscillations are robust against errors at the Ising point, while they become weaker as the transverse field $h$ increases. In Ref. [RMS20] it is discussed how this effect can be understood from the nature of the decay processes involved for each parameter set $\{g, h\}$, but this is out of the scope of the present discussion.

### 5.5 Application II: storage capacity of quantum neural networks

Completely positive and trace preserving maps have been largely studied in the context of quantum information and quantum communication. In this context, the completely positive and trace preserving map is also called a quantum channel or simply a channel. Two fictional characters, Alice and Bob, communicate using the quantum channel and their aim is to send quantum information through a quantum

### 5.5. APPLICATION II: STORAGE CAPACITY OF QUANTUM NEURAL <br> NETWORKS

channel [NC10]. In this sense, information has to be transmitted from one spatial point, corresponding to Alice's position, to another spatial point, corresponding to Bob's position. Attractor quantum neural networks work similarly, but instead of propagating information in space, one is interested in storing certain patterns in time. Intuitively, the storage capacity of an attractor quantum neural network corresponds to how many states or patterns can a certain completely positive and trace preserving map store, as we discuss in Ref. [LGR+21].

Here, we are interested in finding which is the form of the most general quantum evolution $\mathcal{Z}$ that is able to store $d$ orthogonal patterns, where $d$ is the dimension of the Hilbert space. Namely, given a set of pure and orthogonal quantum states $\left\{\rho_{i}=|i \times i|\right\}$ with $i=1, \cdots, d$ corresponding to the patterns that we are interested to store, we want to find non-trivial maps $\mathcal{Z} \neq \mathcal{I}$ such that $\mathcal{Z}[|i \times i|]=|i \times i|$.

The first step is to consider $\rho_{\mathcal{Z}}$ the Jamiołkowski-Choi state of the map $\mathcal{Z}$, which has the general form

$$
\begin{equation*}
\left.\rho_{\mathcal{Z}}=\frac{1}{d} \sum_{i^{\prime} j^{\prime}} \mathcal{Z}\left[\left|i^{\prime} X j^{\prime}\right|\right] \otimes\left|i^{\prime} X j^{\prime}\right|=\frac{1}{d} \sum_{i j i^{\prime} j^{\prime}} \mathcal{Z}_{i j i^{\prime} j^{\prime} \mid i i^{\prime}} X_{j j^{\prime}} \right\rvert\, . \tag{5.43}
\end{equation*}
$$

We rewrite $\mathcal{Z}=\mathcal{I}+\mathcal{Z}-\mathcal{I}$ to obtain the decomposition

$$
\begin{equation*}
\rho_{\mathcal{Z}}=\rho_{I}+\frac{1}{d} \sum_{i j, i^{\prime} j^{\prime}}\left(\mathcal{Z}_{i j i^{\prime} j^{\prime}}-\delta_{i i^{\prime}} \delta_{j j^{\prime}}\right)\left|i i^{\prime} X j j^{\prime}\right|=: \rho_{I}+\frac{1}{d} Q, \tag{5.44}
\end{equation*}
$$

where $\rho_{I}$ is the Jamiołkowski-Choi state of the identity map $\mathcal{I}$, and reads

$$
\begin{equation*}
\rho_{I}=\frac{1}{d} \sum_{i j}|i i \nmid j j| . \tag{5.45}
\end{equation*}
$$

Several properties can be deduced for $Q$ that follow from its definition (5.44) together with the properties of $\rho_{\mathcal{Z}}$. First, the fact that $\rho_{\mathcal{Z}}$ is a non-trivial map implies that $Q \neq 0$. Second, the trace preserving condition implies that $\operatorname{tr}_{\mathrm{B}}\left[\rho_{z}\right]=\operatorname{tr}_{\mathrm{B}}\left[\rho_{I}\right]=\mathbf{1}_{d} / d$, and then $\operatorname{tr}_{\mathrm{B}}[Q]=0$. Crucially, we also observe from the definition of $Q$ that $\left\langle i^{\prime}\right| Q\left|i^{\prime}\right\rangle=0$. Therefore, for $i \neq i^{\prime}$

$$
\begin{equation*}
\left\langle i i^{\prime}\right| \rho_{\mathcal{Z}}\left|i i^{\prime}\right\rangle=\left\langle i i^{\prime}\right| \rho_{I}\left|i i^{\prime}\right\rangle+\frac{1}{d}\left\langle i i^{\prime}\right| Q\left|i i^{\prime}\right\rangle=0 . \tag{5.46}
\end{equation*}
$$

which, in turn, implies that $\rho_{\mathcal{Z}}\left|i i^{\prime}\right\rangle=0$ because $\rho_{\mathcal{Z}} \geq 0$. Then, projecting Eq. (5.44) from the right by $\left|i i^{\prime}\right\rangle$ with $i \neq i^{\prime}$ reveals that

$$
\begin{equation*}
\rho_{\mathcal{Z}}\left|i i^{\prime}\right\rangle=0=Q\left|i i^{\prime}\right\rangle . \tag{5.47}
\end{equation*}
$$

## CHAPTER 5. SPECTRAL PROPERTIES OF QUANTUM EVOLUTIONS

Therefore, we can write $Q$ in the reduced subspace with basis $\{|i i\rangle\}$ with $i=1, \cdots, d$ in such a way that has the matrix representation

$$
\begin{equation*}
Q=\sum_{i j} Q_{i j}|i i \times j j|, \tag{5.48}
\end{equation*}
$$

with $Q_{i j}=Q_{j i}^{*}$ from the Hermiticity of Q , and $Q_{i i}=0$ since $\langle i i| Q|i i\rangle=0$. Thus, we arrive at the final form

$$
\begin{equation*}
\rho_{\mathcal{Z}}=\frac{1}{d} \sum_{i j}\left(1+Q_{i j}\right)|i i \times j j| \geq 0 \tag{5.49}
\end{equation*}
$$

Note that the positivity of the state further restricts $\left|1+Q_{i j}\right| \leq 1$, which follows from imposing that the $i j^{\text {th }}$ minor of the matrix $\rho_{\mathcal{Z}}$ has a positive determinant.

Equation (5.49) corresponds to the most general Jamiołkowski-Choi state of the form of a completely positive and trace preserving map $\mathcal{Z}$ that stores the $d$ orthogonal patterns $\rho_{i}=|i \times i|$ for $i=1, \cdots, d$.

As an example, we consider the case of a single spin- $1 / 2$ particle $\mathcal{H}=\mathbb{C}^{2}$ for which we want to store two orthogonal states $|-\rangle$ and $|+\rangle$. In this basis, the corresponding Jamiołkowski-Choi state is given by

$$
\rho_{\mathcal{Z}}=\frac{1}{2}\left(\begin{array}{cccc}
1 & 0 & 0 & |q| e^{-i \phi}  \tag{5.50}\\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
|q| e^{i \phi} & 0 & 0 & 1
\end{array}\right)
$$

where $q=1+Q_{+-}=|q| \exp (i \phi)$ is a complex number whose modulus $|q| \leq 1$. The diagonalization of $\rho_{\mathcal{Z}}$ gives rise to the Kraus operators

$$
\begin{align*}
& K_{1}=\sqrt{\frac{1+|q|}{2}}\left(\begin{array}{cc}
1 & 0 \\
0 & e^{i \phi}
\end{array}\right),  \tag{5.51}\\
& K_{2}=\sqrt{\frac{1-|q|}{2}}\left(\begin{array}{cc}
1 & 0 \\
0 & -e^{i \phi}
\end{array}\right), \tag{5.52}
\end{align*}
$$

for the canonical map $\mathcal{Z}$.
As a final remark, in [LGR+21] we discuss more extensively how to use the formalism of quantum operations to analyze the storage capacity of quantum attractor neural networks as well as their learning capabilities.

### 5.6 Chapter's outlook

In this chapter we review the spectral properties of completely positive and trace preserving maps, which are close analogues of those of classical stochastic maps. Interestingly, we have seen that the eigenvalues of the so-called dynamical matrix (the vectorized map) lie within the unit disk. However, the dynamical matrix is not the only possible matrix representation of a quantum evolution. A reshuffling of the indices leads to the so-called Jamiołkowski-Choi state, which is a normalized quantum state in a higher dimension space. Interestingly, the eigenvectors of the Jamiołkowski-Choi state are a vectorized form of the Kraus operators.

Knowing that the spectral properties of quantum evolutions inherit important constraints from the conditions of complete positivity and trace preservation, we move to study whether is it possible to characterize quantum evolutions by their spectral properties. We study two examples of such characterization. The first is related to time crystals, an exotic phase of matter that breaks (discrete) time translational symmetry, and the second to the storage capacity of attractor quantum neural networks.

In the next chapter, we take the quantum Langevin equation approach to study the dynamics and thermodynamics of a system of linearly coupled harmonic oscillators.

## Heat transport in harmonic systems

In the weak-coupling master equation description, we have focused on approaching the dynamics of open quantum systems with arbitrary Hamiltonians and requiring a weak coupling with its environment. We now take the complementary strategy. We fix the underlying Hamiltonian description while allowing for arbitrary coupling strengths to the environment. The underlying Hamiltonian description is fixed to be that of quadratic Hamiltonians or, equivalently, linear equations of motion. Taking this approach has, of course, advantages and limitations.

On the positive side, the study of quadratic Hamiltonians allows studying the dynamics of open quantum system beyond the commonly used approximations of weak-coupling and memoryless environments. In fact, the linear structure of the equations of motion allow for an exact analytical solution of the dynamics through an object known as the covariance matrix. Moreover, arbitrarily complicated physical systems that are weakly perturbed out of equilibrium can be "linearized" and modelled using quadratic Hamiltonians. On the downside, of course, this process can disregard important dynamical processes and one has to be careful when extracting conclusions from a linearized dynamics.

Nonetheless, the versatility and transversality of quadratic Hamiltonians has given this approach popularity in a variety of models and applications, from heat transport in ion traps [FMP15], nanomagnetic rigid rotors [RR16], or thermometry [MSC19] to name a few. In this chapter, we closely follow Ref. [RMP+19] to
explore one of such applications, which is closely related to the problem of heat rectification (see for instance [LRW+12]).

In this chapter, we aim at studying the dynamics and thermodynamics of a collection of linearly coupled harmonic oscillators and, in particular, to study the problem of heat rectification in linear systems. To this end, we first introduce the quantum Langevin equation and a method to solve its stationary dynamics. Then, we define the thermodynamic quantities of interest like internal energy, heat, or work. Afterwards, we introduce the problem of heat rectification and analyze it for general harmonic networks. Finally, we quantify the asymmetry of the heat transfer in the harmonic network for a minimal model of two coupled oscillators.

In this chapter, we encounter some unusual notation. For instance, we use the bold face characters to denote vectors of quantum operators, expectation values $\langle\circ\rangle$ are taken with respect to the initial system plus bath state $\rho\left(t_{0}\right)$, and the trace tr is sometimes taken with respect to "usual" matrices and not quantum states. Moreover, we drop the inverse temperature from the bosonic occupation number $n_{v}\left(\beta_{v}, \omega\right) \mapsto n_{v}(\omega)$ for notational simplicity.

### 6.1 The quantum Langevin equation

In this section, we derive the so-called quantum Langevin equation [FKM65; GWT84; Bre07]. To this end, we introduce first a model known as the harmonic network, which corresponds to a collection of harmonic oscillators. Such network is in contact with a set of infinite baths that are initially decorrelated from the system. Then, we derive the equation of motion for the position and momenta of the harmonic network, which is the quantum Langevin equation. Finally, we discuss briefly the fluctuation-dissipation relation for this model.

### 6.1.1 The harmonic network

We start introducing the microscopic description of the open harmonic network. Each node of the network is one of a collection of $N$ linearly-coupled harmonic oscillators with a time-dependent Hamiltonian:

$$
\begin{equation*}
H_{\mathrm{S}}(t)=\frac{\mathbf{p}^{T} M^{-1} \mathbf{p}}{2}+\frac{\mathbf{x}^{T} V(t) \mathbf{x}}{2} \tag{6.1}
\end{equation*}
$$

We assume that the system S is driven periodically; that is, the potential $V(t)=$ $V(t)^{T}=V\left(t+\tau_{\mathrm{d}}\right)$ is a periodic function with period $\tau_{\mathrm{d}}$. In Eq. (6.1), the vector $\mathbf{x}=\left(x_{1}, \cdots, x_{N}\right)^{T}$ collects all position operators of the network, while the vector $\mathbf{p}=$
$\left(p_{1}, \cdots, p_{N}\right)^{T}$ collects all momenta. They fulfill the standard canonical commutation relations $\left[x_{i}, p_{j}\right]=i \delta_{i j}(=1)$. The matrix $M=\operatorname{diag}\left(m_{1}, \cdots, m_{N}\right)$ is a diagonal matrix that gathers all the masses of the harmonic network. The off-diagonal terms of the time-dependent matrix $V(t)$ capture the interaction strength between the oscillators, while its diagonal part encodes their self-energy.

We consider the system $S$ to be coupled to several baths labeled by $v$, being $H_{v}$ the Hamiltonian of the bath $v$. In turn, each bath is described by a collection of non-interacting oscillators $r$, with masses $M_{v}=\operatorname{diag}\left(\left\{m_{v, r}\right\}\right)$ and frequencies $\Omega_{v}=\operatorname{diag}\left(\left\{\Omega_{v, r}\right\}\right)$. The bath Hamiltonian is

$$
\begin{equation*}
H_{v}=\frac{\mathbf{p}_{v}^{T} M_{v}^{-1} \mathbf{p}_{v}}{2}+\frac{\mathbf{x}_{v}^{T} M_{v} \Omega_{v}^{2} \mathbf{x}_{v}}{2} \tag{6.2}
\end{equation*}
$$

where $\mathbf{x}_{v}=\left(\left\{x_{v, r}\right\}\right)^{T}$ and $\mathbf{p}_{v}=\left(\left\{p_{v, r}\right\}\right)^{T}$ are the bath position and momentum vector operators, respectively. The interaction Hamiltonian between the system $S$ and the bath $v$ is given by

$$
\begin{equation*}
H_{\mathrm{int}, v}=-\mathbf{x}^{T} C_{v} \mathbf{x}_{v}, \tag{6.3}
\end{equation*}
$$

where the rectangular matrix $C_{V}$ encodes the coupling strength between the system and the bath $v$. Then, the total Hamiltonian is given by $H=H_{\mathrm{S}}+\sum_{v} H_{\mathrm{int}, v}+\sum_{v} H_{v}$.

We can compute the Heisenberg equations of motion (2.12) for the system and bath degrees of freedom, which in matrix form are

$$
\begin{align*}
& \dot{\mathbf{x}}=M^{-1} \mathbf{p},  \tag{6.4}\\
& \dot{\mathbf{p}}=-V(t) \mathbf{x}+\sum_{v} C_{V} \mathbf{x}_{v},  \tag{6.5}\\
& \dot{\mathbf{x}}_{v}=M_{v}^{-1} \mathbf{p}_{v},  \tag{6.6}\\
& \dot{\mathbf{p}}_{v}=-M_{v} \Omega_{v}^{2} \mathbf{x}_{v}+C_{v}^{T} \mathbf{x}, \tag{6.7}
\end{align*}
$$

where, for compactness, we use the $\dot{\mathbf{x}}$ to denote its total time derivative $\dot{\mathbf{x}}=(d / d t) \mathbf{x}$. We assume that the system S is initially uncorrelated from the environment $\rho\left(t_{0}\right)=$ $\rho_{\mathrm{S}}\left(t_{0}\right) \otimes_{v} \rho_{v}\left(t_{0}\right)$. Then, taking the time derivative of Eq. (6.6), and combining with Eq. (6.7), we end up with a second order differential equation for the position operator $\mathbf{x}_{v}$ of the bath $v$, whose solution yields

$$
\begin{align*}
\mathbf{x}_{v}(t)= & \cos \left[\Omega_{v}\left(t-t_{0}\right)\right] \mathbf{x}_{v}\left(t_{0}\right)+\left(M_{v} \Omega_{v}\right)^{-1} \sin \left[\Omega_{v}\left(t-t_{0}\right)\right] \mathbf{p}_{v}\left(t_{0}\right)+ \\
& +\int_{t_{0}}^{t} \mathrm{~d} t^{\prime}\left(M_{v} \Omega_{v}\right)^{-1} \sin \left[\Omega_{v}\left(t-t^{\prime}\right)\right] C_{v}^{T} \mathbf{x}\left(t^{\prime}\right), \tag{6.8}
\end{align*}
$$

where $\mathbf{x}_{v}\left(t_{0}\right)$ and $\mathbf{p}_{v}\left(t_{0}\right)$ correspond to the initial conditions. In the same manner, by taking the time derivative of Eq. (6.4), and by substituting Eqs. (6.5) and (6.8) into it, we arrive at

$$
\begin{align*}
& M \ddot{\mathbf{x}}+V(t) \mathbf{x}-\sum_{v} \int_{t_{0}}^{t} \mathrm{~d} t^{\prime} C_{v}\left(M_{v} \Omega_{v}\right)^{-1} \sin \left[\Omega_{v}\left(t-t^{\prime}\right)\right] C_{v}^{T} \mathbf{x}\left(t^{\prime}\right) \\
& \quad=\sum_{v} C_{v}\left(\cos \left[\Omega_{v}\left(t-t_{0}\right)\right] \mathbf{x}_{v}\left(t_{0}\right)+\left(M_{v} \Omega_{v}\right)^{-1} \sin \left[\Omega_{v}\left(t-t_{0}\right)\right] \mathbf{p}_{v}\left(t_{0}\right)\right) \tag{6.9}
\end{align*}
$$

Since we are only interested in the steady-state behavior, we take the limit $t_{0} \rightarrow-\infty$, which leads to the quantum Langevin equation

$$
\begin{equation*}
M \ddot{\mathbf{x}}+V(t) \mathbf{x}-(\chi \star \mathbf{x})(t)=\mathbf{B}(t), \tag{6.10}
\end{equation*}
$$

where $\star$ denotes the convolution in the Fourier sense; that is, given two arbitrary functions $f(t)$ and $g(t)$ its convolution is defined as $(f \star g)(t):=\int_{\mathbb{R}} d t^{\prime} f\left(t-t^{\prime}\right) g\left(t^{\prime}\right)$. The susceptibility matrix $\chi(t)$ acts as a damping source, whereas the noise vector $B(t)$ as a "random" external force. Their explicit expressions are

$$
\begin{align*}
& \chi(t)=\theta(t) \sum_{v} C_{v}\left(M_{v} \Omega_{v}\right)^{-1} \sin \left(\Omega_{v} t\right) C_{v}^{T}  \tag{6.11}\\
& \mathbf{B}(t)=\lim _{t_{0} \rightarrow-\infty} \sum_{v} C_{v}\left\{\sin \left[\Omega_{v}\left(t-t_{0}\right)\right] \mathbf{x}_{v}\left(t_{0}\right)+\left(M_{v} \Omega_{v}\right)^{-1} \cos \left[\Omega_{v}\left(t-t_{0}\right)\right] \mathbf{p}_{v}\left(t_{0}\right)\right\} \tag{6.12}
\end{align*}
$$

with $\theta(t)$ being the Heaviside step function, which arises from causality. We also introduce the spectral density matrix for the $v^{\text {th }}$ bath $J_{v}(\Omega)=1 / 2 C_{v}\left(M_{v} \Omega_{v}\right)^{-1} \Delta(\Omega) C_{v}^{T}$, being $[\Delta(\Omega)]_{r r^{\prime}}=\delta_{r r^{\prime}} \delta\left(\Omega-\Omega_{v, r}\right)$. We further assume that all oscillators of the network are at most coupled to one bath. One can think of $J_{\nu}(\Omega)$ as a measure of the number of modes in bath $v$ whose frequencies lie between $\Omega$ and $\Omega+\mathrm{d} \Omega$. With the help of the spectral density, we rewrite $\chi(t)=2 \theta(t) \sum_{v} \int_{0}^{\infty} \mathrm{d} \Omega J_{v}(\Omega) \sin (\Omega t)$. By extending $J(\Omega)$ to negative frequencies as $J_{v}(-\omega):=-J_{v}(\omega)$, it follows that $\operatorname{Im} \chi(\omega)=\pi \sum_{v} J_{v}(\omega)$, which we shall keep in mind.

### 6.1.2 Solution to the quantum Langevin equation

We are only interested in the stationary dynamics of the network. For periodically driven systems, the dynamics is not always stable and, therefore, there is not always a stationary regime. In the following, we assume that such stationary regime exists, and it is independent of the initial conditions of the system [FP17].

We start looking at the easier case of a static harmonic network, for which $V(t)=V_{0}$ is a constant. Then, a particular solution of the quantum Langevin
equation can be found by means of a Fourier transform $\hat{f}(\omega)=\int_{\mathbb{R}} d t f(t) \exp (i \omega t)$. We find that

$$
\begin{equation*}
\hat{\mathbf{x}}(\omega)=\left[-\omega^{2} M+V_{0}-\hat{\chi}(\omega)\right]^{-1} \hat{\mathbf{B}}(\omega)=: \hat{G}_{0}(\omega) \hat{\mathbf{B}}(\omega) . \tag{6.13}
\end{equation*}
$$

where $\hat{G}_{0}(\omega)$ is the static Green's function. Finally, one can transform back to time domain to obtain the stationary solution

$$
\begin{align*}
& \mathbf{x}^{\mathrm{st}}(t)=\int \frac{d \omega}{2 \pi} \hat{G}_{0}(\omega) \hat{\mathbf{B}}(\omega) e^{-i \omega t},  \tag{6.14}\\
& \mathbf{p}^{\mathrm{st}}(t)=-i \int \frac{d \omega}{2 \pi} \omega M \hat{G}_{0}(\omega) \hat{\mathbf{B}}(\omega) e^{-i \omega t} \tag{6.15}
\end{align*}
$$

We remark that here we refer to this solution as "stationary" in the sense that the system has evolved for long enough to forget about the initial conditions. Clearly, $\mathbf{x}^{\text {st }}(t)$ cannot be a constant, since the fluctuating force $\mathbf{B}(t)$ acts on the system at all times.

Let us turn again to the case of a dynamical network with a time-dependent interaction $V(t)=V\left(t+\tau_{\mathrm{d}}\right)$. Let $D(t)[॰]:=M(d / d t)^{2} \circ+V(t) \circ-(\chi \star \circ)(t)$ be the integro-differential operator associated with the quantum Langevin equation. The equation of motion for the dynamical Green's function of this problem is obtained by solving

$$
\begin{equation*}
D(t)\left[G\left(t, t_{0}\right)\right]=M \frac{d^{2} G\left(t, t_{0}\right)}{d t^{2}}+V(t) G\left(t, t_{0}\right)-\int_{\mathbb{R}} d t^{\prime} \chi\left(t-t^{\prime}\right) G\left(t^{\prime}, t_{0}\right)=\delta\left(t-t_{0}\right) 1_{N} \tag{6.16}
\end{equation*}
$$

being $1_{N}$ the $N \times N$ identity matrix. Let $G^{+}\left(t, t_{0}\right)=G\left(t+\tau_{\mathrm{d}}, t_{0}+\tau_{\mathrm{d}}\right)$, which clearly satisfies that $D\left(t+\tau_{\mathrm{d}}\right)\left[G^{+}\left(t, t_{0}\right)\right]=\delta\left(t-t_{0}\right) 1_{N}$. We note that using the properties $d / d t=d / d\left(t+\tau_{\mathrm{d}}\right), V(t)=V\left(t+\tau_{\mathrm{d}}\right)$, and $\left(\chi \star G^{+}\right)(t)=(\chi \star G)\left(t+\tau_{\mathrm{d}}\right)$, we obtain that $D(t)\left[G^{+}\left(t, t_{0}\right)\right]=\delta\left(t-t_{0}\right) 1_{N}$. Therefore, the functions $G\left(t, t_{0}\right)$ and $G^{+}\left(t, t_{0}\right)$ fulfill the same differential equation. Hence, by uniqueness of the solution, both functions are identical $G\left(t, t_{0}\right)=G^{+}\left(t, t_{0}\right)$ in the stationary regime, where the information about the initial conditions is lost.

To solve the quantum Langevin equation in the dynamical case, we exploit the periodicity of the driving. Namely, we define $P(t, \omega):=\int_{\mathbb{R}} d t^{\prime} \exp \left[i \omega\left(t-t^{\prime}\right)\right] G\left(t, t^{\prime}\right)$, which is a periodic function since

$$
\begin{equation*}
P\left(t+\tau_{\mathrm{d}}, \omega\right)=e^{i \omega\left(t+\tau_{\mathrm{d}}\right)} \int_{\mathbb{R}} d t^{\prime} e^{i \omega t^{\prime}} G\left(t+\tau_{\mathrm{d}}, t^{\prime}\right)=P(t, \omega) \tag{6.17}
\end{equation*}
$$

since $G\left(t+\tau_{\mathrm{d}}, t^{\prime}+\tau_{\mathrm{d}}\right)=G\left(t, t^{\prime}\right)$. Thus, we can Fourier expand the periodic functions

$$
\begin{align*}
& V(t)=V\left(t+\tau_{\mathrm{d}}\right)=\sum_{k} V_{k} e^{i k \omega_{\mathrm{d}} t}  \tag{6.18}\\
& P(t, \omega)=P\left(t+\tau_{\mathrm{d}}, \omega\right)=\sum_{k} A_{k}(\omega) e^{i k \omega_{\mathrm{d}}} \tag{6.19}
\end{align*}
$$

where $\omega_{\mathrm{d}}=2 \pi / \tau_{\mathrm{d}}$ is the driving frequency. Since $D(t)$ is a linear operator, we have that

$$
\begin{equation*}
\int_{\mathbb{R}} \mathrm{d} t^{\prime} \exp \left(-i \omega t^{\prime}\right) D(t)\left[G\left(t, t^{\prime}\right)\right]=D(t)[\exp (-i \omega t) P(t, \omega)]=\exp (-i \omega t) 1_{N} \tag{6.20}
\end{equation*}
$$

Thus, using the expansions (6.18) and (6.19), we arrive at

$$
\begin{equation*}
\sum_{k}\left[-M\left(\omega-k \omega_{\mathrm{d}}\right)^{2} e^{i k \omega_{\mathrm{d}} t}+\sum_{j} V_{j} e^{i(j+k) \omega_{\mathrm{d}} t}+\chi\left(\omega-k \omega_{\mathrm{d}}\right) e^{i k \omega_{\mathrm{d}} t}\right] A_{k}(\omega)=1_{N} \tag{6.21}
\end{equation*}
$$

Finally, projecting on the $k^{\text {th }}$ element of the Fourier expansion, one arrives at

$$
\begin{equation*}
\hat{G}_{0}^{-1}\left(\omega-k \omega_{\mathrm{d}}\right) A_{k}(\omega)+\sum_{j \neq 0} V_{j} A_{k-j}(\omega)=\delta_{k, 0} 1_{N}, \tag{6.22}
\end{equation*}
$$

which determines the amplitudes $A_{k}(\omega)$. While a closed form solution for $A_{k}(\omega)$ is rarely available, one can solve self-consistently Eq. (6.22) to obtain

$$
\begin{align*}
& A_{0}(\omega)=\hat{G}_{0}(\omega)+\sum_{j \neq 0} \hat{G}_{0}(\omega) V_{j} \hat{G}_{0}\left(\omega+j \omega_{\mathrm{d}}\right) V_{-j} \hat{G}_{0}(\omega)+\mathcal{O}\left(V_{j}^{4}\right),  \tag{6.23}\\
& A_{k}(\omega)=-\hat{G}_{0}\left(\omega-k \omega_{\mathrm{d}}\right) V_{k} \hat{G}_{0}(\omega)+\mathcal{O}\left(V_{j}^{3}\right), \quad \text { for } k \neq 0 \tag{6.24}
\end{align*}
$$

These are perturbative expansions in terms of the strength of the driving potential $V_{j}$. Such expansions can be seen as a combination of free evolution with interactions with the periodic driving, the latter causing a sudden change of the propagation frequency. This idea is depicted in the diagrams in Fig. 6.1.

Finally, we can use the amplitudes $\left\{A_{k}(\omega)\right\}$ to compute the stationary solution for the dynamical harmonic network

$$
\begin{align*}
& \mathbf{x}^{\mathrm{st}}(t)=\int_{\mathrm{R}} \mathrm{~d} t^{\prime} G\left(t, t^{\prime}\right) \mathbf{B}\left(t^{\prime}\right)=\sum_{k} \int_{\mathrm{R}} \frac{\mathrm{~d} \omega}{2 \pi} A_{k}(\omega) \hat{\mathbf{B}}(\omega) e^{-i\left(\omega-k \omega_{\mathrm{d}}\right) t},  \tag{6.25}\\
& \mathbf{p}^{\mathrm{st}}(t)=\frac{d}{d t} \int_{\mathrm{R}} M G\left(t, t^{\prime}\right) \mathbf{B}\left(t^{\prime}\right)=-i \sum_{k} \int_{\mathrm{R}} \frac{\mathrm{~d} \omega}{2 \pi}\left(\omega-k \omega_{\mathrm{d}}\right) M A_{k}(\omega) \hat{\mathbf{B}}(\omega) e^{-i\left(\omega-k \omega_{\mathrm{d}}\right) t} . \tag{6.26}
\end{align*}
$$



Figure 6.1: Schematic representation of the perturbative expansion of the amplitudes $A_{k}(\omega)$ giving rise to energy exchange processes between the driving and two heat baths with spectral densities $J_{\nu}(\omega)$ and $J_{\mu}(\omega)$.

### 6.1.3 The second moment matrix

Given two observables $X$ and $Y$, we define its second moment as $\langle X Y\rangle$. For a system of $N$ oscillators, the second moment matrix is a $2 N \times 2 N$ matrix, which we divide into the four $N \times N$ blocks

$$
\Sigma(t):=\left(\begin{array}{ll}
\left\langle\mathbf{x x}^{T}\right\rangle & \left\langle\mathbf{x p}^{T}\right\rangle  \tag{6.27}\\
\left\langle\mathbf{p} \mathbf{x}^{T}\right\rangle & \left\langle\mathbf{p p}^{\mathrm{T}}\right\rangle
\end{array}\right),
$$

where, for instance, $\left[\mathbf{x p}^{\mathrm{T}}\right]_{i j}=\left\langle x_{i} p_{j}\right\rangle$. For quadratic Hamiltonians, all the relevant dynamical information can be computed from the first $\langle\mathbf{x}\rangle$ and $\langle\mathbf{p}\rangle$ and second moments encoded in $\Sigma(t)$. Using the stationary solutions in Eq. (6.25) and Eq. (6.26), one can obtain the dynamics of the covariance matrix $\Sigma(t)$. Then, in the stationary regime, all blocks are connected to expectation values of the form $\left\langle\hat{\mathbf{B}}(\omega) \hat{\mathbf{B}}\left(\omega^{\prime}\right)^{T}\right\rangle$. For instance, we find that

$$
\begin{equation*}
\left\langle\mathbf{x}^{\mathrm{st}}(t) \mathbf{x}^{\mathrm{st}}(t)^{T}\right\rangle=\sum_{k k^{\prime}} \iint_{\mathbb{R}} \frac{\mathrm{d} \omega d \omega^{\prime}}{(2 \pi)^{2}} A_{k}(\omega)\left\langle\hat{\mathbf{B}}(\omega) \hat{\mathbf{B}}\left(\omega^{\prime}\right)^{T}\right\rangle A_{k}\left(\omega^{\prime}\right)^{T} e^{-i\left(\omega+\omega^{\prime}-\left(k+k^{\prime}\right) \omega_{\mathrm{d}}\right) t} . \tag{6.28}
\end{equation*}
$$

To proceed on the computation, one has to fix the state $\rho\left(t_{0}\right)$ over which the expectation value is taken, which we do in the following section.

As we will see in the next section, the second moment matrix is also closely related to the thermodynamic quantities of interest, the heat fluxes $\dot{\mathrm{Q}}_{v}$ and the work rate $\dot{W}$.

### 6.2 Thermodynamics of harmonic networks

In this section, we study the thermodynamic properties of the harmonic network. In particular, we focus on the study of heat transport through the harmonic network and, in what follows, we assume that $\rho_{v}\left(t_{0}\right)=\pi_{v}\left(\beta_{v}\right)$ is a thermal state at inverse temperature $\beta_{v}$.

### 6.2.1 Thermodynamic quantities

We start introducing the system internal energy $\mathrm{U}_{\mathrm{S}}:=\left\langle H_{\mathrm{S}}\right\rangle$, for which we obtain

$$
\begin{equation*}
\mathrm{U}_{\mathrm{S}}(t)=\frac{1}{2} \operatorname{tr}\left[M^{-1}\left\langle\mathbf{p} \mathbf{p}^{T}\right\rangle\right]+\frac{1}{2} \operatorname{tr}\left[V(t)\left\langle\mathbf{x} \mathbf{x}^{T}\right\rangle\right], \tag{6.29}
\end{equation*}
$$

To write Eq. (6.29) in "trace form", we have used the property $\left\langle\mathbf{x}^{T} A \mathbf{y}\right\rangle=\sum_{i j} A_{i j}\left\langle x_{i} y_{j}\right\rangle=$ $\operatorname{tr}\left[A^{T}\left\langle\mathbf{x} \mathbf{y}^{T}\right\rangle\right]$, for arbitrary $\mathbf{x}, \mathbf{y}$ and $A$. Note that the internal energy is directly related to the $x x$-block and the $p p$-block of the second moment matrix $\Sigma(t)$.

The next quantity we are interested in is the work rate $\dot{\mathbf{W}}=\partial_{t}\left\langle\operatorname{tr}\left\{\left[\partial_{t} H(t)\right]\right\rangle\right.$, which we defined in Eq. (2.134). Since only $H_{\mathrm{S}}(t)$ depends on time, we can compute the work as

$$
\begin{equation*}
\dot{\mathrm{W}}=\frac{1}{2} \operatorname{tr}\left\{\left[\partial_{t} V(t)\right]\left\langle\mathbf{x} \mathbf{x}^{T}\right\rangle\right\} . \tag{6.30}
\end{equation*}
$$

Using the Heisenberg equation of motion for $H_{\mathrm{S}}(t)$, and taking its average $\langle 0\rangle$ we find that

$$
\begin{equation*}
\frac{d}{d t} \mathrm{U}_{\mathrm{S}}(t)=\sum_{v} i\left\langle\left[H_{\mathrm{int}, v}, H_{\mathrm{S}}(t)\right]\right\rangle+\dot{\mathrm{W}}=: \sum_{v} \dot{\mathrm{Q}}_{v}+\dot{\mathrm{W}} \tag{6.31}
\end{equation*}
$$

which motivates the definition of the local heat flux $\dot{\mathrm{Q}}_{v}:=i\left\langle\left[H_{\mathrm{int}, v}, H_{\mathrm{S}}(t)\right]\right\rangle$ that makes Eq. (6.31) identical the first law. Note, however, that this is an unusual definition for the heat flux, which differs from the more standard

$$
\begin{equation*}
\dot{\mathrm{Q}}_{v}^{\prime}:=-d\left\langle H_{v}\right\rangle / d t=\mathrm{Q}_{v}+\left\langle\left[H_{\mathrm{int}, v}, H_{v}\right]\right\rangle . \tag{6.32}
\end{equation*}
$$

As it turns out, the difference between $\dot{\mathrm{Q}}_{v}$ and $\dot{\mathrm{Q}}_{v}^{\prime}$ is irrelevant for our purposes, while the definition of heat flux $\dot{Q}_{v}$ yields simpler expressions and, thus, we shall stick to it (see App. D.1). We can compute

$$
\begin{equation*}
\dot{\mathrm{Q}}_{v}=\left\langle\mathbf{p}^{T} M^{-1} C_{v} \mathbf{x}_{v}\right\rangle . \tag{6.33}
\end{equation*}
$$

The problem with Eq. (6.33) is that it depends on quantities of the bath $v$. To avoid this, we introduce the projectors $\Pi_{v}$, which project on the sites of the harmonic network that are coupled to the $v^{\text {th }}$ bath. We assume that each oscillator in the network is coupled to at most one bath and, therefore, $\Pi_{\mu} \Pi_{v}=\Pi_{v} \delta_{\mu v}$. Then, we can project Eq. (6.5) to obtain

$$
\begin{equation*}
\dot{\mathrm{Q}}_{v}=\operatorname{tr}\left[\Pi_{v} M^{-1}\left\langle\mathbf{p} \dot{\mathbf{p}}^{T}\right\rangle\right]+\operatorname{tr}\left[\Pi_{v} M^{-1}\left\langle\mathbf{p} \mathbf{x}^{T}\right\rangle V(t)\right] \tag{6.34}
\end{equation*}
$$

which again is connected to blocks of the second moment matrix $\Sigma(t)$. To simplify Eq. (6.34) we use that by definition $\dot{\mathrm{Q}}_{v} \in \mathbb{R}$ and that $\left\langle z_{i} z_{j}\right\rangle=\left\langle z_{j} z_{i}\right\rangle^{\star}$ if $z_{i}$ is Hermitian. We arrive at the final expression

$$
\begin{equation*}
\dot{\mathrm{Q}}_{v}=\frac{1}{2} \operatorname{tr}\left[\Pi_{v} M^{-1} \frac{d}{d t}\left\langle\mathbf{p p}^{T}\right\rangle\right]+\operatorname{tr}\left\{\Pi_{v} M^{-1} V(t) \operatorname{Re}\left[\left\langle\mathbf{x p}^{T}\right\rangle\right]\right\} \tag{6.35}
\end{equation*}
$$

### 6.2.2 Fluctuation-Dissipation Relation

To compute the stationary second moment matrix $\Sigma^{\text {st }}$, we need to often evaluate expectation values of the noise vector $\mathbf{B}(t)$. Here, we perform precisely this computation and show that the result corresponds to a well known form of the fluctuationdissipation theorem. We now take advantage of the initial state $\rho_{v}\left(t_{0}\right)=\pi_{\nu}\left(\beta_{v}\right)$ to perform the calculation. For such thermal state, all first order moments vanish in the stationary regime. Moreover, the second order moments yield:

$$
\begin{align*}
& M_{v} \Omega_{v}\left\langle\mathbf{x}_{v}\left(t_{0}\right) \mathbf{x}_{v}^{T}\left(t_{0}\right)\right\rangle=\left\langle\mathbf{p}_{v}\left(t_{0}\right) \mathbf{p}_{v}^{T}\left(t_{0}\right)\right\rangle\left(M_{v} \Omega_{v}\right)^{-1}=\frac{1}{2} \operatorname{coth}\left(\frac{\beta_{v} \Omega_{v}}{2}\right),  \tag{6.36}\\
& \left\langle\mathbf{x}_{v}\left(t_{0}\right) \mathbf{p}_{v}^{T}\left(t_{0}\right)\right\rangle=\left\langle\mathbf{p}_{v}\left(t_{0}\right) \mathbf{x}_{v}^{T}\left(t_{0}\right)\right\rangle^{*}=\frac{i}{2} . \tag{6.37}
\end{align*}
$$

With these expressions at hand, we are ready to compute the two time expectation value of the noise vector

$$
\begin{equation*}
\left\langle\mathbf{B}(\tau) \mathbf{B}^{T}(0)\right\rangle=\frac{1}{2} \sum_{v} C_{v}\left(M_{v} \Omega_{v}\right)^{-1}\left(\cos \left(\Omega_{v} \tau\right) \operatorname{coth}\left(\frac{\beta_{v} \Omega_{v}}{2}\right)+i \sin \left(\Omega_{v} \tau\right)\right) C_{v}^{T} \tag{6.38}
\end{equation*}
$$

which is only a function of the elapsed time $\tau$. By introducing the spectral density to the last expression, it can be written as

$$
\begin{equation*}
\left\langle\mathbf{B}(\tau) \mathbf{B}(0)^{T}\right\rangle=\sum_{v} \int_{0}^{\infty} \mathrm{d} \Omega J_{v}(\Omega)\left[\cos (\Omega \tau)\left(2 n_{v}(\omega)+1\right)+i \sin (\Omega \tau)\right], \tag{6.39}
\end{equation*}
$$

where $n_{v}(\omega):=\left[\exp \left(\beta_{v} \Omega\right)-1\right]^{-1}$ is the bosonic occupation number of the $v^{\text {th }}$ bath. The real part of the above quantity is known as the noise kernel

$$
\begin{equation*}
\gamma(\tau):=\operatorname{Re}\left[\left\langle\mathbf{B}(\tau) \mathbf{B}(0)^{T}\right\rangle\right]=\sum_{v} \int_{\mathbb{R}} d \omega J(\omega)\left[n_{v}(\omega)+1 / 2\right] e^{-i \omega \tau} . \tag{6.40}
\end{equation*}
$$

which appears very often in the calculations. Finally, the Fourier transformed counterpart of Eq. (6.39) is the well-known fluctuation-dissipation relation

$$
\begin{equation*}
\left\langle\hat{\mathbf{B}}(\omega) \hat{\mathbf{B}}\left(\omega^{\prime}\right)^{T}\right\rangle=\delta\left(\omega+\omega^{\prime}\right)(2 \pi)^{2} \sum_{v} J_{v}(\omega)\left(n_{v}(\omega)+1\right) . \tag{6.41}
\end{equation*}
$$

### 6.2.3 Heat transport in static harmonic networks

We are finally ready to evaluate the heat flux in the stationary regime by putting together the results of Sec. 6.1.3, Sec. 6.2.1 and Sec. 6.2.2.

We start considering the simpler case of a static network, for which $V(t)=V_{0}$ becomes a constant and, then, we have $\dot{W}=0$. In this scenario, the second moment matrix $\Sigma(t) \mapsto \Sigma_{0}^{\text {st }}$ becomes a constant in the stationary regime. The subscript 0 is added to make a clear distinction from the periodically driven network. The time-independence of $\Sigma_{0}^{\text {st }}$ can be checked by direct computation using the noise kernel (6.40). For instance, for the static version of Eq. (6.28) we obtain

$$
\begin{align*}
\left\langle\mathbf{x}^{\mathrm{st}}(t) \mathbf{x}^{\mathrm{st}}(t)^{T}\right\rangle & =\iint d t^{\prime} d t^{\prime \prime} G_{0}\left(t-t^{\prime}\right) \gamma\left(t^{\prime}-t^{\prime \prime}\right) G_{0}\left(t-t^{\prime \prime}\right)^{T} \\
& =\sum_{v} \int_{\mathbb{R}} d \omega \hat{G}_{0}(\omega) J_{v}(\omega) \hat{G}_{0}(\omega)^{\dagger}\left[n_{v}(\omega)+1 / 2\right] . \tag{6.42}
\end{align*}
$$

Because $\Sigma_{0}^{\text {st }}$ is time-independent, the expression of the local heat flux in the stationary regime simplifies into

$$
\begin{equation*}
\left.\dot{\mathrm{Q}}_{v}^{\text {st }}=\operatorname{tr}\left\{\Pi_{v} V_{0} \operatorname{Re}\left[\left\langle\mathbf{x}^{\mathrm{st}}(t) \mathbf{p}^{\mathrm{st}}(t)^{T}\right\rangle\right] M^{-1}\right]\right\} \tag{6.43}
\end{equation*}
$$

We start computing the real part of the $x p$-block of the second moment matrix. Using Eq. (6.39) together with the extension $J_{v}(-\omega)=-J_{v}(\omega)$ we find that

$$
\begin{align*}
\operatorname{Re}\left[\left\langle\mathbf{x}^{\text {st }}(t) \mathbf{p}^{\text {st }}(t)^{T}\right\rangle\right] & =\iint_{\mathbb{R}} d t^{\prime} d t^{\prime \prime} G_{0}\left(t-t^{\prime}\right) \gamma\left(t^{\prime}-t^{\prime \prime}\right) \dot{G}_{0}\left(t-t^{\prime \prime}\right)^{T} M \\
& =\sum_{\mu} \int_{\mathbb{R}} d \omega(i \omega) \hat{G}_{0}(\omega) J_{\mu}(\omega) \hat{G}_{0}(\omega)^{\dagger} M\left[n_{\mu}(\omega)+1 / 2\right] . \tag{6.44}
\end{align*}
$$

where we have used that $\dot{G}_{0}(t)=(2 \pi)^{-1} \int_{\mathbb{R}} d \omega(-i \omega) \hat{G}_{0}(\omega) \exp (-i \omega t)$. Therefore, the stationary heat flux yields

$$
\begin{equation*}
\dot{\mathrm{Q}}_{v}^{\text {st }}=-\sum_{\mu} \int_{\mathbb{R}} d \omega \omega \operatorname{Im}\left\{\operatorname{tr}\left[\Pi_{\nu} V_{0} \hat{G}_{0}(\omega) J_{\mu}(\omega) \hat{G}_{0}(\omega)^{\dagger}\right]\right\}\left[n_{\mu}(\omega)+1 / 2\right] \tag{6.45}
\end{equation*}
$$

We now use Eq. (6.13) to rewrite $V_{0} \hat{G}_{0}(\omega)=1_{N}+\omega^{2} M G_{0}(\omega)+\chi(\omega) G_{0}(\omega)$. Clearly, the only contribution to the heat flux comes from the imaginary part $\operatorname{Im} \chi(\omega)=$ $\pi \sum_{\mu} J_{\mu}(\omega)$. Hence, using $\Pi_{\nu} \operatorname{Im} \chi(\omega)=\pi J_{v}(\omega)$ we arrive at

$$
\begin{equation*}
\dot{\mathrm{Q}}_{v}^{\mathrm{st}}=-\sum_{\mu} \int_{\mathbb{R}} d \omega \pi \omega \operatorname{tr}\left[J_{v}(\omega) \hat{G}_{0}(\omega) J_{\mu}(\omega) \hat{G}_{0}(\omega)^{\dagger}\right]\left[n_{\mu}(\omega)+1 / 2\right] \tag{6.46}
\end{equation*}
$$

which suggests the definition of the static heat transfer matrix

$$
\begin{equation*}
T_{0, v \mu}(\omega):=\pi \omega \operatorname{tr}\left[J_{v}(\omega) \hat{G}_{0}(\omega) J_{\mu}(\omega) \hat{G}_{0}(\omega)^{\dagger}\right] \tag{6.47}
\end{equation*}
$$

Finally, the stationary heat flux can be written into a more convenient form with the help of the first law (6.31). Namely, we have that in the stationary regime $\sum_{\nu} \mathrm{Q}_{\mu}^{\text {st }}=0$, which implies $\sum_{\mu} T_{0, \mu v}(\omega)=0$. Therefore, we have that

$$
\begin{align*}
\dot{\mathrm{Q}}_{v}^{\text {st }}= & -\int_{\mathbb{R}} d \omega T_{0, v v}(\omega)\left[n_{v}(\omega)+1 / 2\right]-\sum_{\mu \neq v} \int_{\mathbb{R}} d \omega T_{0, v \mu}(\omega)\left[n_{\mu}(\omega)+1 / 2\right] \\
& =\sum_{\mu \neq v} \int_{\mathbb{R}} d \omega T_{0, v \mu}(\omega)\left[n_{v}(\omega)-n_{\mu}(\omega)\right], \tag{6.48}
\end{align*}
$$

where we have used that the static heat transfer matrix $T_{0, \mu v}(\omega)=T_{0, v \mu}(\omega)$ is symmetric. This form of the stationary heat fluxs can be found using the nonequilibrium Green's function approach, and we refer to the interested reader to Ref. [DR06] for an extended discussion of the connections between the quantum Langevin equation and nonequilibrium Green's function.

### 6.2.4 Heat transport in dynamic harmonic networks

We consider again a periodically driven harmonic network with a time periodic potential $V(t)=\sum_{k} V_{k} \exp \left(i k \omega_{\mathrm{d}} t\right)$, with Fourier amplitudes $V_{k}$. In this case, the second moment matrix is not constant in the stationary regime. Instead, it adapts to the driving period $\tau_{\mathrm{d}}$, in such a way that $\Sigma^{\text {st }}\left(t+\tau_{\mathrm{d}}\right)=\sum^{\text {st }}(t)$. Again, we can check this property by explicit calculation using Eq. (6.40). For instance, with the help of Eq. (6.25) the $x x$-block yields

$$
\begin{align*}
\left\langle\mathbf{x}^{\mathrm{st}}(t) \mathbf{x}^{\mathrm{st}}(t)^{T}\right\rangle & =\sum_{v} \int d \omega P(t, \omega) J_{\mu}(\omega) P(t, \omega)^{\dagger}\left[n_{v}(\omega)+1 / 2\right] \\
& =\sum_{\mu} \sum_{j k} \int d \omega A_{j}(\omega) J_{\mu}(\omega) A_{k}(\omega)^{\dagger}\left[n_{v}(\omega)+1 / 2\right] e^{i(j-k) \omega_{\mathrm{d}} t}, \tag{6.49}
\end{align*}
$$

which is clearly a periodic function of time.
As a consequence of the periodicity of $\Sigma^{\mathrm{st}}(t)$, the thermodynamic quantities $\dot{\mathrm{Q}}_{v}^{\text {st }}(t)$ and $\dot{\mathrm{W}}^{\text {st }}(t)$ also become time-periodic functions of time in the stationary regime. Thus, we are interested in period-averaged quantities in the stationary regime. We introduce the average over one period

$$
\begin{equation*}
\overline{f(t)}:=\frac{1}{\tau_{\mathrm{d}}} \int_{0}^{\tau_{\mathrm{d}}} d t^{\prime} f\left(t^{\prime}\right) . \tag{6.50}
\end{equation*}
$$

which is constant for any periodic function. A useful property of the average (6.50) is that

$$
\begin{equation*}
\overline{\exp \left[i(j-k) \omega_{\mathrm{d}} t\right]}=\delta_{j k}, \tag{6.51}
\end{equation*}
$$

for $j, k \in \mathbb{Z}$; that is, the functions $\left\{\exp \left[i j \omega_{\mathrm{d}} t\right]\right\}_{j}$ are an orthonormal with respect to the "inner product" $\langle f(t), g(t)\rangle:=\overline{f(t)^{\star} g(t) \text {. }}$

We are now ready to repeat the logic of the last subsection to find the periodaveraged work rate $\overline{\dot{\mathrm{W}}^{\text {stt }}(t)}$ and heat flux $\overline{\dot{\mathrm{Q}}_{v}^{\text {st }}(t)}$. We start by computing the work rate which using Eq. (6.30) yields

$$
\begin{equation*}
\dot{\mathrm{W}}^{\mathrm{st}}(t)=\frac{i}{2} \sum_{\mu} \sum_{j k l} l \omega_{\mathrm{d}} \int d \omega \operatorname{tr}\left[V_{l} A_{j}(\omega) J_{\mu}(\omega) A_{k}(\omega)^{\dagger}\right]\left[n_{\mu}(\omega)+1 / 2\right] e^{i(j-k+l) \omega_{\mathrm{d}} t} \tag{6.52}
\end{equation*}
$$

Then, the period averaged work takes the form

$$
\begin{align*}
\overline{\dot{\mathrm{W}}^{\text {st}}(t)} & =\frac{i}{2} \int d \omega \sum_{\mu} \sum_{j k}(k-j) \omega_{\mathrm{d}} \operatorname{tr}\left[V_{k-j} A_{j}(\omega) J_{\mu}(\omega) A_{k}(\omega)^{\dagger}\right]\left[n_{\mu}(\omega)+1 / 2\right] \\
& =-\int d \omega \sum_{\mu} \sum_{j k} k \omega_{\mathrm{d}} \operatorname{Im}\left\{\operatorname{tr}\left[V_{k-j} A_{j}(\omega) J_{\mu}(\omega) A_{k}(\omega)^{\dagger}\right]\right\}\left[n_{\mu}(\omega)+1 / 2\right], \tag{6.53}
\end{align*}
$$

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where the second line requires splitting the sum into the part proportional to $k \omega_{\mathrm{d}}$ and the one proportional to $j \omega_{\mathrm{d}}$, then exchange the dummy indices $j$ and $k$, and finally use that $V_{k}=V_{-k}^{\dagger}$ to identify the imaginary part of the trace. The expression of the work can be simplified further by noting that Eq. (6.22) implies that

$$
\begin{equation*}
\sum_{j} V_{j} A_{k-j}=\delta_{k, 0} \mathbb{1}+\left(\omega-k \omega_{\mathrm{d}}\right)^{2} M A_{k}(\omega)+\chi\left(\omega-k \omega_{\mathrm{d}}\right) A_{k}(\omega), \tag{6.54}
\end{equation*}
$$

which leads to the final form

$$
\begin{align*}
\overline{\dot{\mathrm{W}}^{\text {st }}(t)} & =\sum_{\mu} \int d \omega \sum_{k} \pi\left(-k \omega_{\mathrm{d}}\right) \operatorname{tr}\left[J\left(\omega-k \omega_{\mathrm{d}}\right) J_{\mu}(\omega) A_{k}(\omega)^{\dagger}\right]\left[n_{\mu}(\omega)+1 / 2\right] \\
& =: \sum_{\mu} \int d \omega \tilde{T}_{\mu}(\omega)\left[n_{\mu}(\omega)+1 / 2\right] . \tag{6.55}
\end{align*}
$$

Next, we proceed to compute the period averaged heat flux in the same manner. We start with computing the $x p$-block of the covariance matrix

$$
\begin{equation*}
\operatorname{Re}\left[\left\langle\mathbf{x}^{\mathrm{st}}(t) \mathbf{p}^{\mathrm{st}}(t)^{T}\right\rangle\right]=\sum_{\mu, j k} \int_{\mathbb{R}} \mathrm{d} \omega i\left(\omega-k \omega_{\mathrm{d}}\right) A_{j}(\omega) J_{\mu}(\omega) A_{k}(\omega)^{\dagger} M\left[n_{\mu}(\omega)+1 / 2\right] e^{i(j-k) \omega_{\mathrm{d}} t} . \tag{6.56}
\end{equation*}
$$

Then, we use this expression in Eq. (6.35), and note that the first term does not contribute since $\left\langle\mathbf{p}^{\text {st }}(t) \mathbf{p}^{\text {st }}(t)^{T}\right\rangle$ is a periodic function of time and, therefore, the period average of its derivative vanishes. Therefore, using Eq. (6.56) leads to

$$
\begin{align*}
\overline{\dot{\mathrm{Q}}_{v}^{\mathrm{st}}}(t) & \left.=\operatorname{tr}\left[\Pi_{v} \overline{V(t) \operatorname{Re}\left[\left\langle\mathbf{x}^{\mathrm{st}}(t) \mathbf{p}^{\mathrm{st} t}(t)^{T}\right\rangle\right.}\right] M^{-1}\right]  \tag{6.57}\\
& =-\sum_{\mu, j k} \int_{\mathrm{R}} \mathrm{~d} \omega\left(\omega-k \omega_{\mathrm{d}}\right) \operatorname{Im}\left\{\operatorname{tr}\left[\Pi_{v} V_{j} A_{k-j}(\omega) J_{\mu}(\omega) A_{k}(\omega)^{\dagger}\right]\right\}\left[n_{\mu}(\omega)+1 / 2\right] .
\end{align*}
$$

Using again Eq. (6.54) to perform the sum over $j$, we can introduce the dynamical heat transfer matrix

$$
\begin{equation*}
T_{\nu \mu}(\omega)=\sum_{k}\left(\omega-k \omega_{\mathrm{d}}\right) \pi \operatorname{tr}\left[J_{v}\left(\omega-k \omega_{\mathrm{d}}\right) A_{k}(\omega) J_{\mu}(\omega) A_{k}(\omega)^{\dagger}\right] \tag{6.58}
\end{equation*}
$$

in order to rewrite the heat flux as

$$
\begin{equation*}
\overline{\mathrm{Q}_{v}^{\mathrm{st}}(t)}:=-\sum_{\mu} \int_{\mathrm{R}} d \omega T_{v \mu}(\omega)\left[n_{\mu}(\omega)+1 / 2\right], \tag{6.59}
\end{equation*}
$$



Figure 6.2: Sketch of a heat rectification setup where a system $S$ with linear interactions $V(t)$ is connected to two reservoirs at inverse fixed temperatures $\beta_{1}$ and $\beta_{2}$ : (top) forward configuration, (bottom) reversed configuration.

In Eq. (6.59), the diagonal terms of the heat transfer matrix can be computed using the first law $\overline{\dot{\mathrm{W}}^{\text {st }}(t)}+\sum_{v} \overline{\mathrm{Q}_{v}^{\mathrm{stt}}(t)}=0$, which implies that $\tilde{T}_{\mu}(\omega)=\sum_{v} T_{v \mu}(\omega)$ with $\tilde{T}_{\mu}(\omega)$ defined in Eq. (6.55). Thus, we arrive at the final result

$$
\begin{align*}
\overline{\mathrm{Q}_{v}^{\mathrm{st}}(t)}= & -\int_{\mathrm{R}} d \omega \tilde{T}_{v}(\omega)\left[n_{v}(\omega)+1 / 2\right] \\
& +\sum_{\mu \neq v} \int_{\mathbb{R}} d \omega\left\{T_{\mu v}(\omega)\left[n_{v}(\omega)+1 / 2\right]-T_{v \mu}(\omega)\left[n_{\mu}(\omega)+1 / 2\right]\right\} . \tag{6.60}
\end{align*}
$$

Hence, using the formalism of the quantum Langevin equation, we are able to compute analytic expressions for the work rate and the heat flux of a periodically driven harmonic network coupled to an arbitrary number of heat baths.

### 6.3 An application: the heat rectifier

To illustrate the potential of periodically driven systems, we consider here the particular problem of a heat rectifier. Rectifiers are physical systems capable of conducting energy asymmetrically, whether in the form of electric, magnetic, or thermal energy. A thermal rectifier, when connected to two thermal baths at different temperatures, conducts heat asymmetrically if the temperatures of the
baths are interchanged. This effect allows for an effective heat dissipation with a suppressed backflow reaction. We can formulate the problem of heat rectification in the harmonic network as follows.

Consider the harmonic network to be coupled to two heat baths $v=1,2$ which are initially found at the fixed inverse temperatures $\beta_{1} \leq \beta_{2}$. In any out-of-equilibrium scenario, the energy of the reservoirs is redistributed through the system in the form of heat fluxs. We say that the harmonic network acts as a heat rectifier if the magnitude of the heat flux depends on the sign of the temperature gradient. Such asymmetric heat flux is conventionally quantified by the so-called rectification coefficient

$$
\begin{equation*}
R\left(\dot{\mathrm{Q}}_{1}, \dot{\mathrm{Q}}_{1}^{r}\right):=\frac{\left|\dot{\mathrm{Q}}_{1}+\dot{\mathrm{Q}}_{1}^{r}\right|}{\max \left(\left|\dot{\mathrm{Q}}_{1}\right|,\left|\dot{\mathrm{Q}}_{1}^{r}\right|\right)} \tag{6.61}
\end{equation*}
$$

where $\dot{\mathrm{Q}}_{1}\left(\dot{\mathrm{Q}}_{1}^{r}\right)$ is the heat flowing into the system from the first reservoir in the forward $\left(\beta_{1} \leq \beta_{2}\right)$ and reversed $\left(\beta_{1}>\beta_{2}\right)$ configuration, respectively. For $\beta_{1} \leq \beta_{2}$, forward and reversed configurations refer to, respectively, negative and positive temperature gradients (see Fig. 3.1). Notice that $0 \leq R\left(\dot{\mathrm{Q}}_{1}, \dot{\mathrm{Q}}_{1}^{r}\right) \leq 2$. The lower bound is achieved for a system that conducts symmetrically: $\dot{\mathrm{Q}}_{1}^{r}=-\dot{\mathrm{Q}}_{1}$, while the upper bound is saturated for heat fluxs that are independent of the sign of the temperature gradient: $\dot{\mathrm{Q}}_{1}=\dot{\mathrm{Q}}_{1}^{r}$. A system that blocks the heat flux in either configuration fulfills $R\left(\dot{\mathrm{Q}}_{1}, 0\right)=R\left(0, \dot{\mathrm{Q}}_{1}^{r}\right)=1$.

Consider first the case of a static network, where the heat flux is given by Eq. (6.48). One obtains that the reversed heat flux is $\dot{Q}_{1}^{\text {st,r }}=-\dot{Q}_{1}^{\text {st }}$, which leads to $R\left(\dot{\mathrm{Q}}_{1}^{\text {st }},-\dot{\mathrm{Q}}_{1}^{\text {st }}\right)=0$. This is true for every geometry of the harmonic network, which is encoded in $V_{0}$, regardless of how asymmetric one tries to make it. Even if the properties of the bath are different; that is, different $J_{v}(\omega)$, the heat flux is conducted symmetrically. Is it possible to attain asymmetric heat fluxes within harmonic systems? The answer is positive, but it requires exploring time-dependent systems.

In the static network, the symmetric heat conduction is inherited from the symmetry of the static heat transfer matrix $T_{0, \mu \nu}(\omega)=T_{0, v \mu}(\omega)$, which allowed to cast the heat flux in the form Eq. (6.34). In Sec. 6.2.4, we have learned that the heat transfer in periodically driven systems leads to an asymmetric heat transfer matrix $T_{\mu \nu}(\omega) \neq T_{\nu \mu}(\omega)$. Therefore, periodically driven systems are, in principle, able to conduct heat asymmetrically.

For a periodically driven network, the numerator of Eq.(6.61), is given by the
absolute value of

$$
\begin{equation*}
\overline{\dot{\mathrm{Q}}_{1}^{\mathrm{st}}(t)}+\overline{\dot{\mathrm{Q}}_{1}^{\text {st,r }}(t)}=-\overline{\dot{\mathrm{W}}_{1}^{\text {st }}(t)}-\overline{\dot{\mathrm{W}}_{1}^{\mathrm{st,r}}(t)}+\int_{\mathrm{R}} \mathrm{~d} \omega\left[T_{21}(\omega)-T_{12}(\omega)\right]\left[n_{1}(\omega)+n_{2}(\omega)+1\right], \tag{6.62}
\end{equation*}
$$

where we have rewritten

$$
\begin{equation*}
\overline{\dot{\mathrm{W}}^{\mathrm{st}}(t)}=\sum_{v} \overline{\dot{\mathrm{~W}}_{v}^{\mathrm{st}}(t)}:=\sum_{v} \int d \omega \tilde{T}_{v}(\omega)\left[n_{v}(\omega)+1 / 2\right] \tag{6.63}
\end{equation*}
$$

being $\overline{\dot{\mathrm{W}}_{v}^{\text {st }}(t)}$ the local work rates.
The notion of a local work rate is unusual, since work is done on the whole harmonic network and it is independent of the heat baths. However, in the stationary regime, we know that the work has to be compensated by the heat fluxes to give rise to the first law. Hence, we give to $\overline{\dot{\mathrm{W}}_{v}^{\text {st }}(t)}$ the following interpretation. Consider a particular cycle of the stationary regime, where an amount of energy $\mathrm{W}\left(\tau_{\mathrm{d}}\right):=\tau_{\mathrm{d}} \sum_{v} \overline{\dot{\mathrm{~W}}_{v}^{s t}(t)}$ has been injected to/extracted from the harmonic network. Because in the stationary regime the period averaged internal energy $\overline{\mathrm{U}_{\mathrm{S}}^{\text {st }}(t)}$ of the harmonic network remains constant, the extra/deficit of energy $\mathrm{W}\left(\tau_{\mathrm{d}}\right)$ cannot be stored in the system, and should be dissipated to the heat baths in the following cycle. Then, the quantity $\overline{\dot{\mathrm{W}}_{v}^{\text {st }}(t)}$ corresponds to the average work dissipated to bath $v$ per unit time.

Heat rectification in periodically driven systems is based on two facts: (i) the work injected into the system is a useful resource to redistribute energy and (ii) periodically driven systems exhibit new asymmetric energy exchange processes that have no analog in static systems. We are mostly interested in (ii) and, in order to study explicitly the asymmetric heat conduction, we define the static quasi currents $\dot{\mathrm{q}}_{v}=\overline{\dot{\mathrm{W}}_{v}^{s t}(t)}+\overline{\dot{\mathrm{Q}}_{v}^{\text {st }}(t)}$, where the contribution of the work has been explicitly singled out. They fulfill the static first law $\dot{\mathrm{q}}_{1}+\dot{\mathrm{q}}_{2}=0$ and, as the driving is turned off, they reduce to the static currents of Eq. (6.48). Then, the rectification coefficient

$$
\begin{equation*}
R\left(\dot{\mathrm{q}}_{1}, \dot{\mathrm{q}}_{1}^{r}\right) \propto\left|\int_{\mathrm{R}} \mathrm{~d} \omega\left[T_{21}(\omega)-T_{12}(\omega)\right]\left[n_{1}(\omega)+n_{2}(\omega)+1\right]\right| . \tag{6.64}
\end{equation*}
$$

is a measure of the asymmetry in the heat transfer matrix.
To clarify the relevance of $R\left(\dot{\mathrm{q}}_{1}, \dot{\mathrm{q}}_{1}^{r}\right)$ we consider the following situation. Notice, that the fact (i) above can be also achieved by introducing a third "work" bath that provides the energy while keeping the setup static. Let us denote $\beta_{3}$ and $n_{3}(\omega)$ the
inverse temperature and thermal occupation number of such work bath. The static currents in direct and reversed configuration read

$$
\begin{array}{r}
\dot{\mathrm{Q}}_{1}^{\text {st }}=\int_{\mathrm{R}} \mathrm{~d} \omega T_{0,12}(\omega)\left[n_{1}(\omega)-n_{2}(\omega)\right]+\int_{\mathbb{R}} \mathrm{d} \omega T_{0,13}(\omega)\left[n_{1}(\omega)-n_{3}(\omega)\right], \\
\dot{\mathrm{Q}}_{1}^{\mathrm{str}}=\int_{\mathrm{R}} \mathrm{~d} \omega T_{0,12}(\omega)\left[n_{2}(\omega)-n_{1}(\omega)\right]+\int_{\mathbb{R}} \mathrm{d} \omega T_{0,13}(\omega)\left[n_{2}(\omega)-n_{3}(\omega)\right] . \tag{6.66}
\end{array}
$$

We now single out the current of the third reservoir and denote it by

$$
\begin{equation*}
\dot{\mathrm{W}}^{\text {st }}:=\dot{\mathrm{Q}}_{3}^{\text {st }}=\int_{\mathbb{R}} \mathrm{d} \omega T_{0,31}(\omega)\left[n_{3}(\omega)-n_{1}(\omega)\right]+\int_{\mathbb{R}} \mathrm{d} \omega T_{0,32}(\omega)\left[n_{3}(\omega)-n_{2}(\omega)\right] . \tag{6.67}
\end{equation*}
$$

The first law can be now written as $\dot{\mathrm{Q}}_{1}^{\text {st }}+\dot{\mathrm{Q}}_{2}^{\text {st }}+\dot{\mathrm{W}}^{\text {st }}=0$. Again, we can think about the local contributions to reservoir $v=1,2$ as $\dot{\mathbf{W}}_{v}^{\text {st }}=\int_{\mathbb{R}} \mathrm{d} \omega T_{0,3 v}(\omega)\left(n_{3}(\omega)-n_{v}(\omega)\right)$. It is clear, that $R\left(\dot{\mathrm{Q}}_{1}^{\text {st }}, \dot{\mathrm{Q}}_{1}^{\text {st,r }}\right) \propto\left|\dot{\mathrm{W}}_{1}^{\text {st }}+\dot{\mathrm{W}}_{1}^{\text {st, }}\right| \neq 0$ under the interchange $\beta_{1} \leftrightarrow \beta_{2}$. However, there is no genuine asymmetric transport happening in the sense that $T_{0,12}(\omega)=T_{0,21}(\omega)$ for a static system. By defining $\dot{\mathrm{q}}_{v}:=\dot{\mathrm{Q}}_{v}^{\text {st }}+\dot{\mathrm{W}}_{v}^{\text {st }}$, we only take into account the genuine contributions to the rectification, such that, in the static case $R\left(\dot{\mathrm{q}}_{v}, \dot{\mathbf{q}}_{v}^{r}\right)=0$. With this intuition, we use $R\left(\dot{\mathrm{q}}_{v}, \dot{\mathbf{q}}_{v}^{r}\right)$ as a measure of the asymmetric transport in the driven network that is present exclusively due to periodic forcing.

### 6.4 A minimal model

To better illustrate the phenomenon of heat rectification in the harmonic network, we consider a minimal model of $N=2$ harmonic oscillators with unit mass $M=1_{2}$ and squared natural frequencies $\omega_{0}^{2} \geq 0$ and $\omega_{0}^{2}+\delta \geq 0$. They interact via a quadratic coupling of the form $c_{0}\left(x_{1}-x_{2}\right)^{2}$ in such a way that

$$
V_{0}=\left(\begin{array}{cc}
\omega_{0}^{2}+c_{0} & -c_{0}  \tag{6.68}\\
-c_{0} & \omega_{0}^{2}+\delta+c_{0}
\end{array}\right) .
$$

The matrix $V_{0}$ is positive and has eigenvalues $\omega_{ \pm}^{2}=\omega_{0}^{2}+c_{0}+(\delta / 2) \pm \sqrt{c_{0}^{2}+(\delta / 2)^{2}}$, where $\omega_{ \pm}$are the normal mode frequencies. We assume that the first oscillation is periodically driven with period $\tau_{\mathrm{d}}$ in the form $V(t)=V_{0}+2 V_{1} \cos \left(\omega_{\mathrm{d}} t\right)$, with

$$
V_{1}=\left(\begin{array}{ll}
\epsilon & 0  \tag{6.69}\\
0 & 0
\end{array}\right) .
$$

where $\epsilon$ is a small driving amplitude.

We consider that the harmonic network is coupled to two identical heat baths with susceptibility matrix $\chi(\omega)=\tilde{\chi}(\omega) 1_{N}$, where $\tilde{\chi}(\omega) \in \mathbb{C}$ is the susceptibility function. We fix the imaginary part of the susceptibility through

$$
\begin{equation*}
\operatorname{Im} \tilde{\chi}(\omega)=\pi \tilde{J}(\omega)=2 j_{0} \omega \frac{\omega_{\mathrm{c}}^{2}}{\omega_{\mathrm{c}}^{2}+\omega^{2}}, \tag{6.70}
\end{equation*}
$$

where $\tilde{J}_{v}(\omega)$ is the spectral density function, $j_{0}$ measures the dissipation strength and $\omega_{\mathrm{c}}$ is a high-frequency cutoff.

We are interested in the total susceptibility function, not only in its imaginary part. To find the real part, we take advantage from the fact that $\tilde{\chi}(t)$ is a causal response; that is, proportional to $\theta(t)$. Hence, the susceptibility function $\tilde{\chi}(\omega)$ is an analytic function of $\omega \in \mathbb{C}$ in the upper-half complex plane. To see this, it is sufficient to have in mind the definition $\tilde{\chi}(t)=(2 \pi)^{-1} \int d \omega \tilde{\chi}(\omega) \exp (-i \omega t)$ and regard $\omega$ as a complex parameter. Consider a closed semicircle contour "SC" of radius $r$ in the upper-half complex plane that goes in the real axis from $-r$ to $+r$, and closes with $\omega(\phi)=r \exp (i \phi)$ with $\phi \in[0, \pi)$. Then, for $t<0$ we have

$$
\begin{equation*}
\lim _{r \rightarrow \infty} \oint_{\mathrm{SC}} \frac{d \omega}{2 \pi} \tilde{\chi}(\omega) e^{-i \omega t}=\lim _{r \rightarrow \infty} \int_{-r}^{r} \frac{d \omega}{2 \pi} \tilde{\chi}(\omega) e^{-i \omega t}+\mathcal{O}\left(e^{r t}\right)=\tilde{\chi}(t<0)=0 \tag{6.71}
\end{equation*}
$$

Now, we can single out a point $\omega \in \mathbb{R}$ to rewrite

$$
\begin{equation*}
0=\oint_{C} d \omega^{\prime} \frac{\tilde{\chi}\left(\omega^{\prime}\right)}{\omega^{\prime}-\omega}=\operatorname{PV} \int d \omega^{\prime} \frac{\tilde{\chi}\left(\omega^{\prime}\right)}{\omega^{\prime}-\omega}-i \pi \tilde{\chi}(\omega) \tag{6.72}
\end{equation*}
$$

for any contour $C$ contained in the upper-half complex plane. Taking the real part of the above equation, we arrive at the so-called Kramers-Kronig relation

$$
\begin{equation*}
\operatorname{Re}[\tilde{\chi}(\omega)]=\frac{1}{\pi} \operatorname{PV} \int d \omega^{\prime} \frac{\operatorname{Im}\left[\tilde{\chi}\left(\omega^{\prime}\right)\right]}{\omega^{\prime}-\omega} \tag{6.73}
\end{equation*}
$$

Equation (6.73) tells us that the real and imaginary part of a causal response in the spectral domain are not independent of each other. Then, a standard complex integral calculation reveals that

$$
\begin{equation*}
\tilde{\chi}(\omega)=2 j_{0} \frac{\omega_{\mathrm{c}}^{2}}{\omega_{\mathrm{c}}-i \omega}, \tag{6.74}
\end{equation*}
$$

which, as expected, is analytic in the upper-half plane.
The next step is founding the static Green's function $G_{0}(\omega)$, which governs the dynamics in the limit of a static network, when $\epsilon \rightarrow 0^{+}$. We have that

$$
\begin{equation*}
\left\{-\omega^{2} 1_{2}+V_{0}-\operatorname{Re}[\tilde{\chi}(\omega)] 1_{2}-i \pi \tilde{J}(\omega) 1_{2}\right\} G_{0}(\omega)=1_{2} \tag{6.75}
\end{equation*}
$$

We assume a large high-frequency cutoff $\omega_{\mathrm{c}}$, so that one can approximate $\operatorname{Re}[\tilde{\chi}(\omega)] \approx$ $2 j_{0} \omega_{c}$, which can be reabsorbed in the frequency $\omega_{0}$. We now want to solve Eq. (6.77). Let us denote by $u_{i}$ with $i= \pm$ the eigenvectors of $V_{0}$, such that $V_{0}=\sum_{i} \omega_{i}^{2} u_{i} u_{i}^{T}$ and $1_{2}=\sum_{i} u_{i} u_{i}^{T}$. Then, the static Green function is found to be

$$
\begin{equation*}
G_{0}(\omega)=\sum_{i} \frac{u_{i} u_{i}^{T}}{\omega_{i}^{2}-\omega^{2}-i \pi \tilde{J}(\omega)} . \tag{6.76}
\end{equation*}
$$

The normal mode vectors $u_{i}$ are real, orthogonal and normalized to one, and therefore can be parametrized with an angle $\varphi$ such that $u_{+}=(\sin (\varphi), \cos (\varphi))$ and $u_{-}=(\cos (\varphi),-\sin (\varphi))$. The angle $\varphi$ is determined as a function of the system parameters as $\tan (2 \varphi)=-2 c 0 / \delta$. Then, we find the static Green's function is explicitly given by

$$
\begin{align*}
G_{0}(\omega)= & \frac{1}{\omega_{-}^{2}-\omega^{2}-i \pi \tilde{J}(\omega)}\left(\begin{array}{cc}
\cos (\varphi)^{2} & -\sin (\varphi) \cos (\varphi) \\
-\sin (\varphi) \cos (\varphi) & \sin (\varphi)^{2}
\end{array}\right) \\
& +\frac{1}{\omega_{+}^{2}-\omega^{2}-i \pi \tilde{J}(\omega)}\left(\begin{array}{cc}
\sin (\varphi)^{2} & \sin (\varphi) \cos (\varphi) \\
\sin (\varphi) \cos (\varphi) & \cos (\varphi)^{2}
\end{array}\right) . \tag{6.77}
\end{align*}
$$

We can use the expression of the static Green's function to evaluate the heat transfer matrix $T_{\mu v}(\omega)$. Because we assume that the system is weakly driven, we will compute it only to first order in $\epsilon$, taking advantage of the expansion (6.23) and (6.24). We find

$$
\begin{align*}
& A_{0}(\omega)_{i j}=G_{0}(\omega)_{i j}+\sum_{j= \pm} G_{0}(\omega)_{i 1} G_{0}\left(\omega+j \omega_{\mathrm{d}}\right)_{11} G_{0}(\omega)_{1 j}+\mathcal{O}\left(\epsilon^{4}\right),  \tag{6.78}\\
& A_{k}(\omega)_{i j}=-\epsilon\left[G_{0}\left(\omega-k \omega_{\mathrm{d}}\right)\right]_{i 1}\left[G_{0}(\omega)\right]_{1 j}+\mathcal{O}\left(\epsilon^{3}\right) . \tag{6.79}
\end{align*}
$$

In principle, combining Eq. (6.77), Eq. (6.78), Eq. (6.79), and Eq. (6.58), we can find an analytic expression for the heat transfer matrix $T_{v \mu}(\omega)$ and an integral form for the heat flux $\overline{\dot{\mathrm{Q}}_{v}^{\text {st }}(t)}$. However, the resulting formula is not very insightful, and it is more instructive to compute numerically the heat flux.

In the top panel of Fig. 6.3, we show the rectification coefficient as a function of the driving frequency $\omega_{d}$ and the coupling constant $c_{0}$. Notice that the driven network reaches $R\left(\overline{\dot{\mathrm{Q}}_{1}^{\text {st }}(t)}, \overline{\dot{\mathrm{Q}}_{1}^{\text {st, }}(t)}\right)=1$, indicating that the heat flux $\overline{\dot{Q}}_{1}$ is completely suppressed in one of the configurations. In fact, such a system even attains $R\left(\overline{\dot{\mathrm{Q}}_{1}^{\text {st }}(t)}, \dot{\mathrm{Q}}_{1}^{\text {st, }}(t)\right) \geq 1$, a regime only possible when the network conducts heat against a thermal gradient in one of the configurations. The regions with non-zero rectification correspond to driving frequencies of $\omega_{\mathrm{d}}=\left\{\omega_{+}-\omega_{-}, 2 \omega_{-}, \omega_{+}+\omega_{-}, 2 \omega_{+}\right\}$.


Figure 6.3: Rectification coefficient as a function of the driving frequency $\omega_{d}$ and the coupling constant $c_{0}$ : (top) using the full current $\dot{\mathrm{Q}}_{1}^{\text {st }}(t)$; (bottom) using the static quasi-current $\dot{q}_{1}$. The black dashed lines lie at the driving frequencies $\omega_{\mathrm{d}}=$ $\left\{\omega_{+}-\omega_{-}, 2 \omega_{-}, \omega_{+}+\omega_{-}, 2 \omega_{+}\right\}$. The parameters are $\delta=\omega_{0}^{2}, j_{0}=0.01 \omega_{0}, \omega_{\mathrm{c}}=10 \omega_{0}$, $\epsilon=0.1 \omega_{0}^{2}, \beta_{1}=\left(1.2 \omega_{0}\right)^{-1}$, and $\beta_{2}=\omega_{0}^{-1}$.

## CHAPTER 6. HEAT TRANSPORT IN HARMONIC SYSTEMS

In the bottom panel of Fig. 6.3, we show the $R\left(\dot{\mathrm{q}}_{1}, \dot{\mathrm{q}}_{1}^{r}\right)$ versus the driving frequency $\omega_{d}$ and the coupling constant $c_{0}$. In comparison with the top panel of Fig. 6.3, we no longer observe the regions of high rectification corresponding to $\omega_{d}=2 \omega_{-}$and $2 \omega_{+}$. This implies that, even though the energy of the bath $v=1$ is kept constant and energy is being injected into the system, no asymmetry of the dynamical heat transfer matrix is achieved. This effect can be understood intuitively by focusing again in the normal mode picture. When the system is driven at frequencies $\omega_{d}=2 \omega_{-}$or $2 \omega_{+}$, the two normal modes remain independent and asymmetric heat exchange is forbidden. However, if the system is driven at $\omega_{d}=\omega_{+} \pm \omega_{-}$, they can interact, enabling asymmetric heat currents. In accordance with the previous discussion, highly asymmetric heat transport occurs at the vicinity of $\omega_{d}=\omega_{+} \pm \omega_{-}$, independently of the driving strength $\epsilon$.

The above results can be understood as follows. In general, a driven harmonic network of $N$ oscillators under consideration is very general, and it is hard to understand a global property such as the heat rectification as a function of the network parameters. However, we can take advantage of the peaked structure of $G_{0}(\omega)$ obtained in Eq. (6.77), and consider only the main contributions to the asymmetric transport in frequency domain. We start using Eq. (6.58) to write

$$
\begin{align*}
T_{21}(\omega)-T_{12}(\omega)= & \sum_{k} \hbar\left(\omega-k \omega_{d}\right) J\left(\omega-k \omega_{d}\right) J(\omega) \pi \epsilon^{2} \\
& \times\left(\left|G_{0}\left(\omega-k \omega_{d}\right)_{21} G_{0}(\omega)_{11}\right|^{2}-\left|G_{0}\left(\omega-k \omega_{d}\right)_{11} G_{0}(\omega)_{12}\right|^{2}\right) . \tag{6.80}
\end{align*}
$$

Therefore, highly asymmetric heat transport can only occur when the two numbers $\left|G_{0}\left(\omega-k \omega_{d}\right)_{21} G_{0}(\omega)_{11}\right|^{2}$ and $\left|G_{0}\left(\omega-k \omega_{d}\right)_{11} G_{0}(\omega)_{12}\right|^{2}$ are large compared with the static transport. The Green's function $G_{0}(\omega)$ is peaked at the normal mode frequencies $\pm \omega_{i}$. Hence, the principal contributions to the asymmetric transport occur when $\omega-k \omega_{\mathrm{d}}$ and $\omega$ correspond to a normal mode frequency $\pm \omega_{i}$ simultaneously. However, notice that when $i=j$ we are evaluating $\left|G_{0}\left(v_{i}\right)_{21} G_{0}\left(v_{i}\right)_{11}\right|^{2}-\left|G_{0}\left(v_{i}\right)_{11} G_{0}\left(v_{i}\right)_{12}\right|^{2}=0$ and consequently the rectification is small. Therefore, only at $k \omega_{d}= \pm \omega_{i} \pm \omega_{j}$ with $i \neq j$, the asymmetric heat transport is expected to be large. In the particular, if we go back to the case of $N=2$, the positive driving frequencies at which one expects large rectification are $\omega_{d}=\omega_{+} \pm \omega_{-}$, as we have observed in Fig. 6.3.

### 6.5 Chapter's outlook

The dynamics of physical systems can be profoundly modified by a time periodic perturbation. A fascinating example of this is the Kapitza pendulum. A static pendulum has a single equilibrium position where its center of mass is at its lowest
height. However, in the Kapitza pendulum one drives periodically the pendulum giving rise to a new stable equilibrium position where the center of mass is at its maximum height! In this chapter, we have exploited a similar idea to obtain asymmetric stationary heat transport in a harmonic network.

We have started introducing the formalism of the quantum Langevin equation to describe the exact open system dynamics of a collection of harmonic oscillators that we refer to as the harmonic network. Then, we have defined internal energy, heat, and work to find that any static (non-driven) network gives rise to vanishing asymmetric currents as quantified by the rectification coefficient. Then, we have considered the case of the periodically driven harmonic network and shown that the asymmetric transport can be different from zero in that case. Finally, we have applied those general idea to a minimal model of only two oscillators. There, we have seen that asymmetric transport occurs when the frequency of the driving is resonant with the sum or difference of the normal mode frequencies of the network. Intuitively, in only in that case that the driving induces an effective interaction between the two normal modes, making possible the heat transport.

## 7

## Conclusions and Outlook

In this thesis we have studied the dynamics of open quantum systems that are in or out of equilibrium. In particular, in the first part of the thesis, we have developed a new master equation approach that goes beyond the Born-Markov-secular paradigm. The motivation for this is as follows. The miniaturization of quantum experiments towards the microscale is often accompanied by a more detailed description of its surroundings. This new available information can potentially be used to predict more accurately the dynamics of open quantum systems. Moreover, for a finite environment, this extra information evolves dynamically and, therefore, it is timely to develop new techniques that can take advantage of this fact. Our master equation approach, the extended microcanonical master equation, takes advantage of this fact by including a dynamically evolving bath and keeping track of the system-bath correlations at a coarse-grained level. We are now in the position to give a concise answer to the theoretical questions (TQ1)-(TQ4), that we posed at the beginning of this thesis.
(TQ1) What does our approach reveal about open quantum system dynamics?
The answer is part of the output of Chap. 3. The extended microcanonical master equation opens up the possibility to describe the dynamics of open quantum systems that interact with a finite, and therefore, dynamically evolving bath. In those systems, the open system generates a non-negligible influence on the bath, causing
it to dynamically evolve by, for instance, building up system-bath correlations or generating nonequilibrium features in the bath. Contrary to the infinite bath paradigm, the global system-bath reaches an equilibrium state that maximizes the total (observational) entropy. That is, in opposition to the system evolving to reach the equilibrium temperature of the bath, which maximizes its local entropy, while leaving the bath "untouched".

## (TQ2) How does our approach connect to previously used techniques?

Also this answer is part of the output of Chap. 3. Consider the generator of the Born-Markov-secular master equation as a function of the inverse temperature of the bath thermal state. We can now ask: which is the time-dependent value of the inverse temperature $\beta$ that makes the dynamics of the Born-Markov-secular master equation as close as possible to the one of the extended microcanonical master equation for the reduced state of the system? Answering this question is in general hard. However, we were able to give an answer to this question in the limit in which the system-bath correlations are small and where the rates that enter the extended microcanonical master equation are a slowly varying function of the energy. In that case, the optimal choice of the inverse temperature corresponds to a nonequilibrium effective inverse temperature $\beta^{\star}(t)$ that interpolates in a hierarchy between the two master equation approaches, and it is in one to one correspondence with the bath average energy. Moreover, from the definition of $\beta^{\star}(t)$, it follows that only a heat bath with an infinite canonical heat capacity has a constant value for the effective nonequilibrium inverse temperature $\beta^{\star}(t)=\beta_{0}$.
(TQ3) Is it possible to complement our approach with a nonequilibrium thermodynamic framework?

The short answer is yes, it is possible, as we have extensively discussed throughout Chap. 4. Namely, we have seen that it is possible to give thermodynamic definitions for the thermodynamic quantities (like internal energy, work, heat, or entropy) such that the laws of thermodynamics arise from the underlying quantum mechanical description. For instance, the total energy of the system plus the coarse-grained energy of the bath is conserved under the dynamics of the extended microcanonical master equation, which ultimately gives rise to the first law. Or, also, we have seen that the total system plus bath observational entropy always increases, which gives rise to the second law. We briefly discuss how one can extend those result to study transport scenarios, in which there is more than one heat bath, although we do not give the explicit thermodynamic treatment in this more general case.
(TQ4) What does this new thermodynamic framework reveal?
One of the most interesting outputs of the discussion in Chap. 4, is that we found a hierarchy of second laws, which is analogous to the hierarchy of master equations obtained in Chap. 3. The first element in the hierarchy states that the change in global observational entropy increases, which follows from the use of the extended microcanonical master equation. From it, we obtain a second law in the form of Clausius inequality, with a time dependent effective inverse temperature given by $\beta^{\star}(t)$. Finally, in the limit of an infinite heat capacity, one can replace the $\beta^{\star}(t)$ by its initial value $\beta_{0}$ to obtain the Clausius inequality for an infinite bath.

As it turns out, the use of Clausius inequality at a constant temperature $\beta_{0}$ has been used to compute the entropy production even for finite baths. We show that taking this approach always leads to higher entropy production or, for the case of thermal machines, a lower efficiency.

In the second part of the thesis, we have move forward weak-coupling master equations, and we have studied other approaches to the dynamics of open quantum systems. The first approach that we consider is the framework of quantum operations, which we use to study general spectral properties of the evolution of open quantum systems. We review the known fact that the completely positive and trace preserving conditions of a quantum evolution implies that the spectrum of the dynamical matrix is contained in the unit disk of the complex plane. Also, after reshuffling the indices of the dynamical matrix one obtains the so-called Jamiołkowski-Choi state, and we also see that its eigenvectors are related to a vectorized form of the Kraus operators. With this information at hand, we proceed to investigate the practical questions (PQ1) and (PQ2).
(PQ1) Can the spectral properties of a quantum evolution give information about (dynamical) phases of matter?

Again, the short answer is yes, as we discuss in Chap. 5. There, we study a dynamical phase of matter known as open discrete time crystals, which can only occur in periodically driven systems. This phase of matter is characterized by displaying robust subharmonic oscillations that last, ideally, up to infinite time. The idea is that if such a phase of matter can exist, these properties must be reflected on the spectrum of the corresponding dynamical matrix. For instance, given that at least two states are visited at stroboscopic times in the long time limit, at least two eigenvalues must lie in the unit circle. Moreover, if the subharmonic oscillations correspond to the usual period doubling, this phase of matter can be detected by
having an eigenvalue equal to minus one, which shows that this dynamical phase of matter can be detected by analyzing the spectrum of the corresponding quantum evolution.
(PQ2) Which is the general form of a quantum evolution (operation) that leaves invariant a collection of pure states?

As we discuss in Chap. 5, the most general quantum operation that leaves invariant a collection of pure states (patterns) with as many elements as the dimension of the Hilbert space has a very sparse dynamical matrix which has as eigenvectors the populations and coherences of the patterns. While this result may not be surprising, the fact that can be proved within the framework of quantum operations is an example of the potential of this approach.

Finally, we explore the quantum Langevin equation. We have use this approach to study the stationary thermodynamics in periodically driven harmonic networks. This study has led to the answer to the practical question (PQ3).
(PQ3) Is it possible to achieve asymmetric heat transport through a harmonic network?

As we discuss in Chap. 6, the heat transport in static harmonic networks is always symmetric, in the sense that reversing the temperature bias always leads to a global minus sign in the heat current. However, this ceases to be true for periodically driven networks. The heat exchange processes enabled by the periodic driving give rise to a heat exchange asymmetry that we quantify in terms of the rectification coefficient.

To conclude, we have extensively studied a variety of approaches to the dynamics of open quantum systems that are able to describe equilibrium and non equilibrium scenarios. We hope that the theory developed in the first part of this thesis can be extended and combined with existing techniques to explore the intriguing world of finite baths, or to give more accurate predictions about open quantum system dynamics. Also, we also hope that the applications studied in the second part of this thesis may serve as inspiration for further research or, at least, be regarded as original applications of the preexisting theory.

## Technicalities chapter 2

## A. 1 Exact perturbation expansions for the NakajimaZwanzig equation

In this section, we find an exact solution for the Nakajima-Zwanzig equation for a weakly perturbed Hamiltonian $H=H_{0}+\lambda V$ in the form of a perturbation series in powers of a small parameter $\lambda$.

Solutions of the Nakajima-Zwanzig master equation are conveniently found in terms of the Laplace transform, which for the density matrix reads

$$
\begin{equation*}
\hat{\rho}(s)=\int_{0}^{\infty} d t \rho(t) e^{-s t} . \tag{A.1}
\end{equation*}
$$

Then, the Liouville-von Neumann equation (2.62) takes the simple form

$$
\begin{equation*}
s \hat{\rho}(s)-\rho(0)=\mathcal{L} \hat{\rho}(s), \tag{A.2}
\end{equation*}
$$

which leads to the solution

$$
\begin{equation*}
\hat{\rho}(s)=\frac{1}{s-\mathcal{L}} \rho(0) . \tag{A.3}
\end{equation*}
$$

In many cases of interest, the Liouville operator can be decomposed as an unperturbed part $\mathcal{L}_{0}$ and a perturbation $\mathcal{L}_{1}$; that is, $\mathcal{L}=\mathcal{L}_{0}+\lambda \mathcal{L}_{1}$. Then, one can take advantage of the identity

$$
\begin{equation*}
\frac{1}{s-\mathcal{L}}=\frac{1}{s-\mathcal{L}_{0}}+\frac{1}{s-\mathcal{L}_{0}} \lambda \mathcal{L}_{1} \frac{1}{s-\mathcal{L}^{\prime}} \tag{A.4}
\end{equation*}
$$

to obtain perturbative expansions in the parameter $\lambda$. Equation (A.4) is nothing else than the Laplace transform of Eq. (??) for $X=\mathcal{L}$ and $Y=\mathcal{L}_{0}$. The Laplace transform of the Kernel is

$$
\begin{equation*}
\hat{\mathcal{K}}(s)=\mathcal{P} \mathcal{L} \frac{1}{s-\mathcal{Q L}} \mathcal{Q} \mathcal{L}=\mathcal{P} \mathcal{L} \frac{1}{s-\mathcal{Q} \mathcal{L}_{0}} \sum_{n=0}^{\infty} \lambda^{n}\left[\mathcal{Q} \mathcal{L}_{1} \frac{1}{s-\mathcal{Q} \mathcal{L}_{0}}\right]^{n} \mathcal{Q} \mathcal{L} . \tag{A.5}
\end{equation*}
$$

We now see that the lowest order solution of the Kernel $n=0$ corresponds to weak-coupling master equations, which are second order in $\lambda$. Specifying further the relevant map $\mathcal{P}$ often leads to further simplifications of $\hat{\mathcal{K}}(s)$, but we do not discuss this here. Similarly, the inhomogenous term in Laplace space is

$$
\begin{equation*}
\hat{I}(s)=\mathcal{P} \mathcal{L} \frac{1}{s-\mathcal{Q} \mathcal{L}_{0}} \sum_{n=0}^{\infty} \lambda^{n}\left[\mathcal{Q} \mathcal{L}_{1} \frac{1}{s-\mathcal{Q} \mathcal{L}_{0}}\right]^{n} \mathcal{Q} \rho(0) . \tag{A.6}
\end{equation*}
$$

With those expressions at hand, the full solution of the Nakajima-Zwanzig equation is simply

$$
\begin{equation*}
\mathcal{P} \hat{\rho}(s)=\frac{1}{s-\mathcal{P} \mathcal{L}-\hat{\mathcal{K}}(s)}[\mathcal{P} \rho(0)+\hat{I}(s)], \tag{A.7}
\end{equation*}
$$

which is of no practical use.

## A. 2 More about the Markov approximation

The derivation of the master equations presented in Sec. 2.2 is rigorous. Nonetheless, the Markovian approximation requires further discussion. Here, we discuss the close relationship between the Markov approximation and the infinite bath limit.

First, taking the limit $t \rightarrow \infty$ in Eq. (2.49) is only justified if the integrand converges sufficiently quickly to zero. However, the bath correlation functions cannot decay for arbitrary long times if the bath has a discrete spectrum. This result is known as the quantum Poincaré recurrence theorem. The proof of the quantum recurrence theorem requires mathematical notions of the theory of quasi-periodic

## APPENDIX A. TECHNICALITIES CHAPTER 2

functions [BL57]. Physical intuition about the recurrences can be obtained as follows.

For simplicity, we take the bath correlation functions with $\alpha=\alpha^{\prime}$. To show that the bath correlation function has recurrences, we need to show that $\mid C_{\alpha \alpha}(\mathbf{a} ; \tau)-$ $C_{\alpha \alpha}(\mathbf{a} ; 0) \mid$ is bounded from above for an arbitrarily small parameter $\epsilon$. We first write

$$
\begin{align*}
\left|C_{\alpha \alpha}(\mathbf{a} ; \tau)-C_{\alpha \alpha}(\mathbf{a} ; 0)\right| & =\left.\left|\sum_{k q}\right|\left[\delta B_{\alpha}(\mathbf{a})\right]_{q k}\right|^{2}\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]_{k k}\left(e^{i\left(e_{k}-e_{q}\right) \tau}-1\right) \mid \\
& \leq 2 \sum_{k q}\left|\left[\delta B_{\alpha}(\mathbf{a})\right]_{q k}\right|^{2}\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]_{k k}\left(1-\cos \left[\left(e_{k}-e_{q}\right) \tau\right]\right) . \tag{A.8}
\end{align*}
$$

We define a small frequency $\delta \omega$ such that $e_{k}-e_{q}=\left(n_{k q}+\epsilon_{k q}\right) \delta \omega$ with $\epsilon_{k q} \ll 1$ and $n_{k q} \in \mathbb{Z}$. Also, consider the long time $\tau=\tau(\delta \omega)=2 \pi / \delta \omega$. Then,

$$
\begin{align*}
\left|C_{\alpha \alpha}(\mathbf{a} ; \tau)-C_{\alpha \alpha}(\mathbf{a} ; 0)\right| & \approx(2 \pi)^{2} \sum_{k q}\left|\left[\delta B_{\alpha}(\mathbf{a})\right]_{q k}\right|^{2}\left|\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]_{k k}\right| \epsilon_{k q}^{2} \\
& \leq(2 \pi)^{2} M_{\alpha}(\mathbf{a}) \sum_{i}\left[\Phi_{\mathrm{B}}(\mathbf{a})\right]_{k k} \sum_{q} \epsilon_{k q}^{2}, \tag{A.9}
\end{align*}
$$

where $M_{\alpha}(\mathbf{a}):=\max _{q k}\left|\left[\delta B_{\alpha}(\mathbf{a})\right]_{q k}\right|^{2}$. Similarly, we introduce the $\epsilon:=\sqrt{\max _{k} \sum_{q} \epsilon_{k q}^{2}}$. Hence, we arrive at

$$
\begin{equation*}
\left|C_{\alpha \alpha}(\mathbf{a} ; \tau)-C_{\alpha \alpha}(\mathbf{a} ; 0)\right| \lesssim(2 \pi)^{2} M_{\alpha}(\mathbf{a}) \epsilon^{2} \tag{A.10}
\end{equation*}
$$

where $\epsilon$ can be made arbitrarily small for an arbitrarily small choice of $\delta \omega$. Similar arguments hold for the case $\alpha \neq \alpha^{\prime}$. Hence, the integrals $\Gamma_{\alpha \alpha^{\prime}}(\mathbf{a} ; \omega)$ do not converge.

The situation is very different if the bath has a continuous spectrum; that is, if the bath has an uncountable infinite number of frequencies. The reason is the Riemann-Lebesgue lemma, which stands that given an absolutely integrable function $\hat{f}(\omega)$, then

$$
\begin{equation*}
\lim _{\tau \rightarrow \infty} f(\tau)=\lim _{\tau \rightarrow \infty} \int \frac{d \omega}{2 \pi} \hat{f}(\omega) e^{-i \omega \tau}=0 \tag{A.11}
\end{equation*}
$$

The proof is as follows. Let the indicator function $1_{[a, b]}(\omega)=1$ if $\omega \in[a, b]$ and $1_{[a, b]}(\omega)=0$ else. For any $\hat{f}(\omega)$ it exists an arbitrarily good approximation $\hat{h}(\omega)=$ $\sum_{i} h_{i} 1_{\left[a_{i} b_{i}\right]}(\omega)$ with arbitrary coefficients $h_{i} \in \mathbb{C}$ and $a_{i}, b_{i} \in \mathbb{R}$, such that

$$
\begin{equation*}
\int d \omega|\hat{f}(\omega)-\hat{h}(\omega)| \leq 2 \pi \epsilon \tag{A.12}
\end{equation*}
$$

where $\epsilon \geq 0$ is arbitrarily small. Moreover, the function $\hat{h}(\omega)$ fulfills the condition

$$
\begin{equation*}
\lim _{\tau \rightarrow \infty} h(\tau):=\lim _{\tau \rightarrow \infty} \int \frac{d \omega}{2 \pi} \hat{h}(\omega) e^{i \omega \tau}=\sum_{i} \frac{h_{i}}{2 \pi} \lim _{\tau \rightarrow \infty} \frac{e^{i b_{i} \tau}-e^{i a_{i} \tau}}{i \tau}=0 . \tag{A.13}
\end{equation*}
$$

Then, we arrive at

$$
\begin{equation*}
\lim _{\tau \rightarrow \infty}|\hat{f}(\omega)| \leq \int \frac{d \omega}{2 \pi}|\hat{f}(\omega)-\hat{h}(\omega)|+\lim _{\tau \rightarrow \infty}\left|\int \frac{d \omega}{2 \pi} \hat{h}(\omega) e^{i \omega \tau}\right| \leq \epsilon . \tag{A.14}
\end{equation*}
$$

which is arbitrarily small and, therefore, proves the initial claim. A similar statement holds for square integrable functions [RH12].

Consider now the absolutely integrable operator $\delta \hat{B}_{\alpha}(\mathbf{a} ; \omega)$ that fulfills

$$
\begin{equation*}
\int \frac{d \omega}{2 \pi} \delta \hat{B}_{\alpha}(\mathbf{a} ; \omega)=\delta B_{\alpha}(\mathbf{a}) \tag{A.15}
\end{equation*}
$$

Then the function $\hat{f}(\omega)=\left\langle\delta \hat{B}_{\alpha}(\mathbf{a} ; \omega)^{\dagger} \delta B_{\alpha}(\mathbf{a})\right\rangle_{\mathbf{a}}$ is also integrable since

$$
\begin{equation*}
\int \frac{d \omega}{2 \pi} \hat{f}(\omega)=\left\langle\delta B_{\alpha}(\mathbf{a})^{\dagger} \delta B_{\alpha}(\mathbf{a})\right\rangle_{\mathbf{a}}<+\infty \tag{A.16}
\end{equation*}
$$

Then, the correlation function yields

$$
\begin{equation*}
\lim _{\tau \rightarrow \infty} C_{\alpha \alpha}(\mathbf{a} ; \tau)=\lim _{\tau \rightarrow \infty} \int \frac{d \omega}{2 \pi} \hat{f}(\omega) e^{i \omega \tau}=0 \tag{A.17}
\end{equation*}
$$

and the decay of the correlation function to zero is guaranteed by the RiemannLebesgue lemma.

To conclude, the Markov approximation is well justified in two different scenarios. The first one corresponds to considering times $t$ are much smaller than the typical recurrence time, albeit, much larger than the bath correlation time $\tau_{\mathrm{B}}$. The second, corresponds to taking the infinite bath limit which, intuitively, pushes the recurrence time to infinity.

## Technicalities chapter 3

## B. 1 Useful properties EMME projectors

We divide the Liouvillian as follows $\mathcal{L}=\mathcal{L}_{0, \mathrm{~S}}+\mathcal{L}_{0, \mathrm{~B}}+\lambda \mathcal{L}_{1}$, where $\mathcal{L}_{0, \mathrm{~S}}[\circ]=-i\left[H_{\mathrm{S}},{ }^{\circ}\right]$, $\mathcal{L}_{0, \mathrm{~B}}[\circ]=-i\left[H_{\mathrm{B}}, \circ\right]$, and $\mathcal{L}_{1}[\circ]=\mathcal{L}^{\mathrm{mf}}+\mathcal{L}_{V}=-i \lambda^{-1} \sum_{x}\left[H_{\mathrm{S}}^{\mathrm{mf}}\left(E_{x}\right) \otimes \Pi\left(E_{x}\right), \circ\right]-i[V, \circ \cdot]$. We note the properties

$$
\begin{align*}
& \mathcal{P} \mathcal{L}_{0, \mathrm{~S}}=\mathcal{L}_{0, \mathrm{~S}} \mathcal{P}=-i\left[H_{\mathrm{S}}, \sum_{x} \operatorname{tr}\left[\Pi\left(E_{x}\right) \circ\right] \otimes \omega_{\mathrm{B}}\left(E_{x}\right)\right],  \tag{B.1}\\
& \mathcal{P}_{0, \mathrm{~B}}=\mathcal{L}_{0, \mathrm{~B}} \mathcal{P}=0,  \tag{B.2}\\
& \lambda \mathcal{P} \mathcal{L}^{\mathrm{mf}}=\lambda \mathcal{L}^{\operatorname{mf} \mathcal{P}} \boldsymbol{\mathcal { P }}=-i \sum_{x}\left[H_{\mathrm{S}}^{\operatorname{mf}}\left(E_{x}\right), \operatorname{tr}_{\mathrm{B}}\left[\Pi\left(E_{x}\right)^{\circ}\right] \otimes \omega_{\mathrm{B}}\left(E_{x}\right)\right],  \tag{B.3}\\
& \lambda \mathcal{P} \mathcal{L}_{V}=-i \lambda \sum_{x} \operatorname{tr}_{\mathrm{B}}\left[\Pi\left(E_{x}\right)[V, \circ]\right] \otimes \omega_{\mathrm{B}}\left(E_{x}\right),  \tag{B.4}\\
& \lambda \mathcal{L}_{V} \mathcal{P}=-i \lambda \sum_{x}\left[V, \operatorname{tr}_{\mathrm{B}}\left[\Pi\left(E_{x}\right)^{\circ}\right] \otimes \omega_{\mathrm{B}}\left(E_{x}\right)\right],  \tag{B.5}\\
& \lambda \mathcal{P} \mathcal{L}_{V} \mathcal{P}=0 . \tag{B.6}
\end{align*}
$$

which also show that $\left[\mathcal{Q}, \mathcal{L}_{0}\right]=\left[\mathcal{P}, \mathcal{L}_{0}\right]=0$.

## B. 2 Equivalence Nakajima-Zwanzig and the timelocal equation

In this section, we show the non-trivial correspondance between the second order Nakajima-Zwanzig equation and the time-local equation. Let $\mathcal{P}$ be the relevant map, and $\mathcal{Q}=\mathcal{I}-\mathcal{P}$ be its complementary. Let $H=H_{0}+\lambda V$, where $H_{0}$ is zeroth order in the coupling strength $\lambda$. In the interaction picture with respect to $H_{0}$, the corresponding Liouville-von Neumann equation yields

$$
\begin{equation*}
\partial_{t} \tilde{\rho}(t)=-i \lambda[\tilde{V}(t), \tilde{\rho}(t)]=: \mathcal{L}(t)[\tilde{\rho}(t)] . \tag{B.7}
\end{equation*}
$$

Then, the Nakajima-Zwanzig equation (2.67) applies. Expanding such equation to second order in $\lambda$ we arrive at

$$
\begin{align*}
\partial_{t} \mathcal{P} \tilde{\rho}(t)= & \mathcal{P} \mathcal{L}(t) \mathcal{P} \tilde{\rho}(t)+\mathcal{P} \mathcal{L}(t) \mathcal{Q} \tilde{\rho}(0) \\
& +\mathcal{P} \mathcal{L}(t) \int_{0}^{t} d t^{\prime} \mathcal{Q} \mathcal{L}\left(t^{\prime}\right) \mathcal{Q} \tilde{\rho}(0)+\mathcal{P} \mathcal{L}(t) \int_{0}^{t} d t^{\prime} \mathcal{Q} \mathcal{L}\left(t^{\prime}\right) \mathcal{P} \tilde{\rho}\left(t^{\prime}\right) . \tag{B.8}
\end{align*}
$$

We want to manipulate Eq. (B.8) to make contact with the alternative derivation in the main text. First, note that the formal integration of the Liouville-von Neumann equation and left multiplication by $\mathcal{P}$ gives

$$
\begin{equation*}
\mathcal{P} \tilde{\rho}(t)=\mathcal{P} \tilde{\rho}(0)+\mathcal{P} \int_{0}^{t} d t^{\prime} \mathcal{L}\left(t^{\prime}\right) \tilde{\rho}\left(t^{\prime}\right) . \tag{B.9}
\end{equation*}
$$

Substituting $\mathcal{P} \tilde{\rho}(t)$ into Eq. (B.8) and rearranging yields

$$
\begin{align*}
\partial_{t} \mathcal{P} \tilde{\rho}(t)= & \mathcal{P} \mathcal{L}(t) \tilde{\rho}(0)+\mathcal{P} \mathcal{L}(t) \int_{0}^{t} d t^{\prime} \mathcal{L}\left(t^{\prime}\right) \tilde{\rho}\left(t^{\prime}\right) \\
& +\mathcal{P} \mathcal{L}(t) \int_{0}^{t} d t^{\prime} \mathcal{Q} \mathcal{L}\left(t^{\prime}\right)\left[\mathcal{Q} \tilde{\rho}(0)-\mathcal{Q} \tilde{\rho}\left(t^{\prime}\right)\right] \tag{B.10}
\end{align*}
$$

where the rightmost term can be ignored since the difference $\mathcal{Q} \tilde{\rho}(0)-\mathcal{Q} \tilde{\rho}\left(t^{\prime}\right)$ is of order $\lambda$. Interestingly, there is a much simpler way to arrive to Eq. (B.10). The formal solution of the Liouville-von Neumann Eq. (B.7) reads

$$
\begin{equation*}
\tilde{\rho}(t)=\tilde{\rho}(0)+\int_{0}^{t} d t^{\prime} \mathcal{L}(t) \tilde{\rho}(0)+\int_{0}^{t} d t^{\prime} \int_{0}^{t^{\prime}} d t^{\prime \prime} \mathcal{L}\left(t^{\prime}\right) \mathcal{L}\left(t^{\prime \prime}\right) \tilde{\rho}\left(t^{\prime \prime}\right) \tag{B.11}
\end{equation*}
$$

After taking the derivative of the above equation we get

$$
\begin{equation*}
\partial_{t} \tilde{\rho}(t)=\mathcal{L}(t) \tilde{\rho}(0)+\mathcal{L}(t) \int_{0}^{t} d t^{\prime} \mathcal{L}\left(t^{\prime}\right) \tilde{\rho}\left(t^{\prime}\right) \tag{B.12}
\end{equation*}
$$

which after acting with $\mathcal{P}$ from the left is identical to Eq. (B.10) to second order in the coupling strength $\lambda$.

In conclusion, we have proven that it is equivalent to use the second-order expansion of the Nakajima-Zwanzig equation or the time-local equation as a starting point to derive a second order master equation for the relevant degrees of freedom $\mathcal{P} \rho$ even in the case where $\mathcal{P}^{2} \neq \mathcal{P}$.

## B. 3 The Lindeberg theorem

In probability theory, the Lindeberg theorem provides a sufficient condition for a set of random variables to converge to a normal distribution. We present here the details showing that Lindeberg theorem guarantees the convergence of the density of states $g(e)$ of the spin bath to a normal distribution.

The Lindeberg theorem is as follows. Let $X_{N, r}$ be a triangular array of independent (but not necessarily identically distributed) random variables where $r=1, \cdots, N$, with $\mathbb{E}\left[X_{N, r}\right]=0$ and $\mathbb{E}\left[X_{N, r}^{2}\right]=\sigma_{N, r}^{2}$. Define the random variable of the $\operatorname{sum} S_{N}:=\sum_{r=1}^{N} X_{N, r}$ with $\mathbb{E}\left[S_{N}\right]=0$ and $\mathbb{E}\left[S_{N}^{2}\right]=\sigma_{N}^{2}:=\sum_{r=1}^{N} \sigma_{N, r}^{2}$. If the Lindeberg condition

$$
\begin{equation*}
\lim _{N \rightarrow \infty} \frac{1}{\sigma_{N}^{2}} \sum_{r=1}^{N} \mathbb{E}\left[X_{N, r}^{2}:\left|X_{N, r}\right|>\epsilon \sigma_{N}\right]=0 \quad \forall \epsilon>0, \tag{B.13}
\end{equation*}
$$

holds, then, $S_{N}$ is normally distributed with zero mean and standard deviation $\sigma_{N}$ as $N$ tends to infinity.

The application to the spin bath is as follows. Consider a spin bath of $N$ noninteracting spin $-1 / 2$ particles. A bath eigenstate $\left|e_{\mathbf{n}}\right\rangle$ is uniquely identified by the sequence $\mathbf{n}=\left(n_{1}, \cdots, n_{N}\right)$ where $n_{r}=\{-1,+1\}$ are independent and identically distributed random variables with probability $p( \pm 1)=1 / 2$, with associated mean $\mathbb{E}\left[n_{r}\right]=0$ and variance $\mathbb{E}\left[n_{r}^{2}\right]=1 / 4$. However, the individual contribution to the energy is scaled by a prefactor $\Omega_{r} / 2>0$, so we define $X_{N, r}=n_{r} \Omega_{r} / 2$. We note that

$$
\begin{align*}
\sum_{r=1}^{N} \mathbb{E}\left[X_{N, r}^{2}:\left|X_{N, r}\right|>\epsilon \sigma_{N}\right] & =\sum_{r=1}^{N} \Omega_{r}^{2} \mathbb{E}\left[n_{r}^{2}:\left|n_{r}\right|>\Omega_{r}^{-1} \epsilon \sigma_{N}\right] \\
& =\left(\sum_{r=1}^{N} \Omega_{r}^{2}\right) \mathbb{E}\left[n_{1}^{2}:\left|n_{1}\right|>\left\{\max _{r} \Omega_{r}\right\}^{-1} \epsilon \sigma_{N}\right] \tag{B.14}
\end{align*}
$$

where we have used the independent and identically distribution for the $n_{r}$ 's. Hence,
the Lindeberg condition holds provided that

$$
\begin{equation*}
\lim _{N \rightarrow \infty} \frac{\max _{r} \Omega_{r}}{\sqrt{\sum_{r} \Omega_{r}^{2} / 4}}=0 \tag{B.15}
\end{equation*}
$$

which we assume to be true for our spin bath. Therefore, we obtain a Gaussian density of states $g(e)=2^{N} \mathcal{N}\left(e, \sigma_{N}\right)$.

## Technicalities chapter 5

## C. 1 Matrix inequality in an extended space

In this appendix, we want to prove the following equivalence between matrix inequalities. Consider $X, Y, Z$ to be $d \times d$ matrices, with $X>0$. Then,

$$
S_{\mathrm{c}}[A]:=Z-Y^{\dagger} X^{-1} Y \geq 0 \Leftrightarrow A:=\left(\begin{array}{cc}
X & Y  \tag{C.1}\\
Y^{\dagger} & Z
\end{array}\right) \geq 0 .
$$

where the combination $S_{\mathrm{c}}[A]$ is also known as the Schur complement. The proof is as follows. First, a quick calculation reveals that

$$
\left(\begin{array}{cc}
X & 0  \tag{C.2}\\
0 & S_{\mathrm{c}}[A]
\end{array}\right)=\left(\begin{array}{cc}
\mathbf{1}_{d} & -X^{-1} Y \\
0 & \mathbf{1}_{d}
\end{array}\right)^{\dagger}\left(\begin{array}{cc}
X & Y \\
Y^{\dagger} & Z
\end{array}\right)\left(\begin{array}{cc}
\mathbf{1}_{d} & -X^{-1} Y \\
0 & \mathbf{1}_{d}
\end{array}\right) .
$$

We moreover note that

$$
T:=\left(\begin{array}{cc}
\mathbf{1}_{d} & 0  \tag{C.3}\\
-Y^{\dagger} X^{-1} & \mathbf{1}_{d}
\end{array}\right)=\left(\begin{array}{cc}
\mathbf{1}_{d} & 0 \\
Y^{\dagger} X^{-1} & \mathbf{1}_{d}
\end{array}\right)^{-1} .
$$

is an invertible matrix. Then, given a matrix $A$ and an invertible matrix $T$, one has that $A \geq 0$ if and only if $T^{\dagger} A T \geq 0$, since for every state $|\psi\rangle$ it exists another
state $|\phi\rangle=T^{-1}|\psi\rangle$, such that $|\psi\rangle=T|\phi\rangle$. Moreover, a block-diagonal matrix $T^{\dagger} A T$ is positive $T^{\dagger} A T \geq 0$ if and only if each of the diagonal blocks is positive; that is, $X \geq 0$ and $S_{\mathrm{c}}[A] \geq 0$, which proves our original claim (C.1).

## C. 2 Perturbation theory for maps

In order to assess the robustness of an eigenvalue, we want to consider that given a map $\mathcal{Z}(\epsilon)=\mathcal{Z}+\epsilon \mathcal{V}$, the first order dependence of the eigenvalues $z(\epsilon)$ in $\epsilon$. Here, we give a recipe to compute all the dependence of $z(\epsilon)$ in $\epsilon \ll 1$ in terms of an infinite series. The spectral equation of the map yields,

$$
\begin{align*}
& \langle\langle L(\epsilon)| \mathcal{Z}(\epsilon)=\langle\langle L(\epsilon)| z(\epsilon),  \tag{С.4}\\
& \mathcal{Z}(\epsilon)|R(\epsilon)\rangle\rangle=z(\epsilon)|R(\epsilon)\rangle\rangle, \tag{C.5}
\end{align*}
$$

for a particular eigenvalue $z(\epsilon)$. We assume that $R(\epsilon), L(\epsilon)$ and $z(\epsilon)$ can be expanded in powers of $\epsilon$

$$
\begin{align*}
& \left.|R(\epsilon)\rangle\rangle=\sum_{k \geq 0} \epsilon^{k}\left|R^{(k)}\right\rangle\right\rangle,  \tag{C.6}\\
& \left\langle\langle L(\epsilon)|=\sum_{k \geq 0} \epsilon^{k}\left\langle\left\langle L^{(k)}\right|,\right.\right.  \tag{C.7}\\
& z(\epsilon)=\sum_{k \geq 0} \epsilon^{k} z^{(k)} . \tag{C.8}
\end{align*}
$$

Using the above expansions into the eigenvalue equation (C.5), it follows that

$$
\begin{equation*}
\left.\left.\left.\left.\left.\mathcal{Z}\left|R^{(0)}\right\rangle\right\rangle+\sum_{k \geq 1} \epsilon^{k}\left(\mathcal{Z}\left|R^{(k)}\right\rangle\right\rangle+\mathcal{V}\left|R^{(k-1)}\right\rangle\right\rangle\right)=\sum_{k \geq 1} \sum_{l=1}^{k} \epsilon^{k} z^{(l)}\left|R^{(k-l)}\right\rangle\right\rangle+\sum_{k \geq 0} z^{(0)} \epsilon^{(k)}\left|R^{(k)}\right\rangle\right\rangle . \tag{C.9}
\end{equation*}
$$

Because the expansion has to be equal order by order in $\epsilon$, we obtain the recurrence relation

$$
\begin{equation*}
\left.\left.\left.\left(\mathcal{Z}-\epsilon^{(0)}\right)\left|R^{(k)}\right\rangle\right\rangle=\mathcal{V}\left|R^{(k-1)}\right\rangle\right\rangle-\sum_{l=1}^{k} z^{(l)}\left|R^{(k-l)}\right\rangle\right\rangle . \tag{C.10}
\end{equation*}
$$

The correction to the eigenvalues can be computed by projecting onto $\left\langle\left\langle L^{(0)}\right|\right.$, which leads to

$$
\begin{equation*}
\left.z^{(k)}=\left\langle\left\langle L^{(0)}\right| \mathcal{Z} \mid R^{(k-1)}\right\rangle\right\rangle-\sum_{l=1}^{k-1} z^{(l)}\left\langle\left\langle L^{(0)} \mid R^{(k-l)}\right\rangle\right\rangle=\frac{1}{k!}\left[\frac{\partial^{k} z(\epsilon)}{\partial \epsilon^{k}}\right]_{\epsilon=0} \tag{C.11}
\end{equation*}
$$

## APPENDIX C. TECHNICALITIES CHAPTER 5

Finally, the first order correction is computed from the simple equation

$$
\begin{equation*}
\left.z^{(1)}=\left[\partial_{\epsilon} z(\epsilon)\right]_{\epsilon=0}=\left\langle\left\langle L^{(0)}\right| \mathcal{Z} \mid R^{(0)}\right\rangle\right\rangle, \tag{C.12}
\end{equation*}
$$

which is the expression used in the main text.
As a final remark, perturbed eigenvectors can be also computed from Eq. (C.10), however its expression is quite involved and dependent on the choice of the inverse of the operator $\mathcal{Z}-\epsilon^{(0)}$ [LPK14] and we do not include them here.

## Technicalities chapter 6

## D. 1 Equivalence of the heat currents

In Chap. 2 and Chap. 3, we have argued that the correct definition of the heat flux that comes from the bath $v$ corresponds to

$$
\begin{align*}
\dot{\mathrm{Q}}_{v}^{\prime}: & =-\operatorname{tr}\left\{H_{v}\left[\partial_{t} \rho\right]\right\}=\operatorname{tr}\left\{\left(H_{\mathrm{S}}(t)+H_{\mathrm{int}, v}\right)\left[\partial_{t} \rho\right]\right\}=\operatorname{tr}\left[\left(H_{S}(t)+H_{S R_{v}}\right) \dot{\rho}(t)\right] \\
& =\dot{\mathrm{Q}}_{v}-\delta \dot{\mathrm{Q}}_{v}, \tag{D.1}
\end{align*}
$$

where we have used that $\operatorname{tr}\left\{H(t)\left[\partial_{t} \rho(t)\right]\right\}=0$, and defined $\delta \dot{\mathrm{Q}}_{v}=\dot{\mathrm{Q}}_{v}-\dot{\mathrm{Q}}_{v}^{\prime}$ as the difference between the heat flux $\dot{\mathrm{Q}}_{v}$ defined in the main text and the standard definition $\mathrm{Q}_{v}^{\prime}$. Equivalently, using the equation of motion for $\rho(t)$, we can recast the difference as

$$
\begin{equation*}
\delta \dot{\mathrm{Q}}_{v}=i\left\langle\left[H_{\mathrm{int}, v}, H_{\mathrm{S}}(t)+H_{v}\right]\right\rangle=-i\left\langle\left[H(t), H_{\mathrm{int}, v}\right]\right\rangle . \tag{D.2}
\end{equation*}
$$

Now, using the Heisenberg equation of motion for $H_{\text {int }, v}$ and rewriting it in terms of the vector operators we arrive at

$$
\begin{equation*}
\delta \dot{Q}_{v}=\frac{d}{d t}\left\langle\mathbf{x}^{T} C_{v} \mathbf{x}_{v}\right\rangle=\frac{d}{d t}\left\langle\mathbf{x}^{T} \Pi_{v}\left(\frac{d \mathbf{p}}{d t}+V(t) \mathbf{x}\right)\right\rangle . \tag{D.3}
\end{equation*}
$$

In the stationary regime, we can compute the two summands in Eq. (D.3) using the same techniques displayed in the main text, to arrive at the conclusion that $\delta \dot{\mathbf{Q}}_{v}^{\text {st }}$ is the time derivative of a time periodic function. More explicitly

$$
\begin{align*}
& \left\langle\mathbf{x}^{T} \Pi_{v} \frac{d \mathbf{p}}{d t}\right\rangle^{s t}=\sum_{j k} K_{1}(j, k) e^{i(j-k) \omega_{d} t},  \tag{D.4}\\
& \left\langle\mathbf{x}^{T} \Pi_{v} V(t) \mathbf{x}\right\rangle^{s t}=\sum_{j l k} K_{2}(j, l, k) e^{i(j+l-k) \omega_{d} t} . \tag{D.5}
\end{align*}
$$

where the functions $K_{1}\left(k, k^{\prime}\right)$ and $K_{2}\left(j, k, k^{\prime}\right)$ are time-independent, and its explicit expression is not important. Therefore, the right-hand-side of Eq. (D.3) is the timederivative of a periodic function of period $\tau_{\mathrm{d}}$, whose contribution over a period averages to zero $\overline{\delta \dot{Q}^{\text {st }}(t)}=0$ which make the two definitions equivalent for periodic drivings in the stationary regime.

## Bibliography

[Cla65] R. Clausius, "Ueber verschiedene für die anwendung bequeme formen der hauptgleichungen der mechanischen wärmetheorie", Ann. Phys. (Berlin) 201, 353-400 (1865).
[Bol77] L. Boltzmann, Über die beziehung zwischen dem zweiten hauptsatze des mechanischen wärmetheorie und der wahrscheinlichkeitsrechnung, respective den sätzen über das wärmegleichgewicht (Kk Hof-und Staatsdruckerei, 1877).
[Pla01] M. Planck, "Über das gesetz der energieverteilung im normalspectrum", Ann. Phys. (Berlin) 309, 553-563 (1901).
[Ein17] A. Einstein, "Zur quantentheorie der strahlung", Phys. Z. 18, 124 (1917).
[Pau28] W. Pauli, "Festschrift zum 60", Geburtstage A. Sommerfelds 30 (1928).
[Neu29] J. von Neumann, "Beweis des ergodensatzes und desh-theorems in der neuen mechanik", Z. Phys. 57, 30-70 (1929).
[Ons31a] L. Onsager, "Reciprocal relations in irreversible processes. i.", Phys. Rev. 37, 405-426 (1931).
[Ons31b] L. Onsager, "Reciprocal relations in irreversible processes. ii.", Phys. Rev. 38, 2265-2279 (1931).
[NLU40] A. Nordsieck, W. Lamb, and G. Uhlenbeck, "On the theory of cosmicray showers i the furry model and the fluctuation problem", Physica 7, 344-360 (1940).
[AP53] A. Abragam and R. V. Pound, "Influence of electric and magnetic fields on angular correlations", Phys. Rev. 92, 943-962 (1953).
[WB53] R. K. Wangsness and F. Bloch, "The dynamical theory of nuclear induction", Phys. Rev. 89, 728-739 (1953).
[Van54] N. Van Kampen, "Quantum statistics of irreversible processes", Physica 20, 603-622 (1954).
[Sol55] I. Solomon, "Relaxation processes in a system of two spins", Phys. Rev. 99, 559-565 (1955).
[BL57] P. Bocchieri and A. Loinger, "Quantum recurrence theorem", Phys. Rev. 107, 337-338 (1957).
[Red57] A. G. Redfield, "On the theory of relaxation processes", IBM J. Res. Dev. 1, 19-31 (1957).
[Van57] L. Van Hove, "The approach to equilibrium in quantum statistics: a perturbation treatment to general order", Physica 23, 441-480 (1957).
[Nak58] S. Nakajima, "On quantum theory of transport phenomena: steady diffusion", Prog. Theor. Phys. 20, 948-959 (1958).
[Zwa60] R. Zwanzig, "Ensemble method in the theory of irreversibility", J. Chem. Phys. 33, 1338-1341 (1960).
[PR61] I. Prigonine and P. Résibois, "On the kinetics of the approach to equilibrium", Physica 27, 629-646 (1961).
[Rés61] P. Résibois, "On the approach to equilibrium in quantum systems", Physica 27, 541-570 (1961).
[SMR61] E. C. G. Sudarshan, P. M. Mathews, and J. Rau, "Stochastic dynamics of quantum-mechanical systems", Phys. Rev. 121, 920-924 (1961).
[Zwa61] R. Zwanzig, Statistical mechanics of irreversibility, Vol. 3 (Interscience New York, 1961), pp. 106-141.
[Mon62] E. Montroll, Fundamental problems in statistical mechanics, 1962.
[Swe62] R. J. Swenson, "Derivation of generalized master equations", J. Math. Phys. 3, 1017-1022 (1962).
[FV63] R. Feynman and F. Vernon, "The theory of a general quantum system interacting with a linear dissipative system", Ann. Phys. 24, 118-173 (1963).
[Rés63] P. Résibois, "On the equivalence between two generalized master equations", Physica 29, 721-741 (1963).
[AK64] P. N. Argyres and P. L. Kelley, "Theory of spin resonance and relaxation", Phys. Rev. 134, A98-A111 (1964).
[Zwa64] R. Zwanzig, "On the identity of three generalized master equations", Physica 30, 1109-1123 (1964).
[FKM65] G. W. Ford, M. Kac, and P. Mazur, "Statistical mechanics of assemblies of coupled oscillators", J. Math. Phys. 6, 504-515 (1965).
[Kra71] K. Kraus, "General state changes in quantum theory", Ann. Phys. 64, 311-335 (1971).
[GRF72] W. M. Gelbart, S. A. Rice, and K. F. Freed, "Random matrix theory and the master equation for finite systems", J. Chem. Phys. 57, 4699-4712 (1972).
[Jam72] A. Jamiołkowski, "Linear transformations which preserve trace and positive semidefiniteness of operators", Rep. Math. Phys. 3, 275-278 (1972).
[AKE73] J. R. Ackerhalt, P. L. Knight, and J. H. Eberly, "Radiation reaction and radiative frequency shifts", Phys. Rev. Lett. 30, 456-460 (1973).
[Aga73] G. S. Agarwal, "Master equation methods in quantum optics", in Prog. Opt. Vol. 11 (Elsevier, 1973), pp. 1-76.
[Haa73] F. Haake, "Statistical treatment of open systems by generalized master equations", in Springer tracts Mod. Phys. (Springer, 1973), pp. 98-168.
[Dav74] E. B. Davies, "Markovian master equations", Comm. Math. Phys. 39, 91-110 (1974).
[Cho75] M.-D. Choi, "Completely positive linear maps on complex matrices", Linear Algebra Appl. 10, 285-290 (1975).
[KM75] H. J. Kimble and L. Mandel, "Problem of resonance fluorescence and the inadequacy of spontaneous emission as a test of quantum electrodynamics", Phys. Rev. Lett. 34, 1485-1488 (1975).
[Dav76] E. B. Davies, Quantum theory of open systems (Academic Press, 1976).
[Gau76] M. Gaudin, "Diagonalization of a class of spin hamiltonians", J. Phys. France 37, 1087-1098 (1976).
[GKS76] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan, "Completely positive dynamical semigroups of n-level systems", J. Math. Phys. 17, 821825 (1976).
[Lin76] G. Lindblad, "On the generators of quantum dynamical semigroups", Comm. Math. Phys. 48, 119-130 (1976).
[Mus77] W. Muschik, "Empirical foundation and axiomatic treatment of nonequilibrium temperature", Arch. Ration. Mech. Anal. 66, 379-401 (1977).
[MB77] W.Muschik and G. Brunk, "A concept of non-equilibrium temperature", Int. J. Eng. Sci. 15, 377-389 (1977).
[Ali79] R. Alicki, "The quantum open system as a model of the heat engine", J. Phys. Math. Gen. 12, L103-L107 (1979).
[DS79] R. Dümcke and H. Spohn, "The proper form of the generator in the weak coupling limit", Z. Phys., B Condens. Matter 34, 419-422 (1979).
[Lin79] G. Lindblad, "Non-markovian quantum stochastic processes and their entropy", Comm. Math. Phys. 65, 281-294 (1979).
[CL83] A. Caldeira and A. Leggett, "Path integral approach to quantum brownian motion", Physica A 121, 587-616 (1983).
[GWT84] H. Grabert, U. Weiss, and P. Talkner, "Quantum theory of the damped harmonic oscillator", Z. Phys., B Condens. Matter 55, 87-94 (1984).
[Yur84] B. Yurke, "Use of cavities in squeezed-state generation", Phys. Rev. A 29, 408-410 (1984).
[CWL85] E. Cortes, B. J. West, and K. Lindenberg, "On the generalized langevin equation: classical and quantum mechanical a)", J. Chem. Phys. 82, 2708-2717 (1985).
[GC85] C. W. Gardiner and M. J. Collett, "Input and output in damped quantum systems: quantum stochastic differential equations and the master equation", Phys. Rev. A 31, 3761-3774 (1985).
[TK89] Y. Tanimura and R. Kubo, "Time evolution of a quantum system in contact with a nearly gaussian-markoffian noise bath", J. Phys. Soc. Japan 58, 101-114 (1989).
[SSO92] A. Suárez, R. Silbey, and I. Oppenheim, "Memory effects in the relaxation of quantum open systems", J. Chem. Phys. 97, 5101-5107 (1992).
[Car93] H. J. Carmichael, "Quantum trajectory theory for cascaded open systems", Phys. Rev. Lett. 70, 2273-2276 (1993).
[Fis98] M. Fischetti, "Theory of electron transport in small semiconductor devices using the pauli master equation", J. Appl. Phys. 83, 270-291 (1998).
[GN99] P. Gaspard and M. Nagaoka, "Slippage of initial conditions for the redfield master equation", J. Chem. Phys. 111, 5668-5675 (1999).
[GZ00] C. W. Gardiner and P. Zoller, Quantum noise (Springer Berlin Heidelberg, 2000).
[PS00] N. V. Prokof'ev and P. C. E. Stamp, "Theory of the spin bath", Rep. Prog. Phys. 63, 669-726 (2000).
[BP02] H.-P. Breuer and F. Petruccione, The theory of open quantum systems (Oxford University Press, 2002).
[EG03] M. Esposito and P. Gaspard, "Quantum master equation for a system influencing its environment", Phys. Rev. E 68, 066112 (2003).
[BGM06] H.-P. Breuer, J. Gemmer, and M. Michel, "Non-markovian quantum dynamics: correlated projection superoperators and hilbert space averaging", Phys. Rev. E 73, 016139 (2006).
[Bud06] A. A. Budini, "Lindblad rate equations", Phys. Rev. A 74, 053815 (2006).
[DR06] A. Dhar and D. Roy, "Heat transport in harmonic lattices", J. Stat. Phys. 125, 801-820 (2006).
[GLT+06] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, "Canonical typicality", Phys. Rev. Lett. 96, 050403 (2006).
[PSW06] S. Popescu, A. J. Short, and A. Winter, "Entanglement and the foundations of statistical mechanics", Nat. Phys. 2, 754-758 (2006).
[Bre07] H.-P. Breuer, "Non-markovian generalization of the lindblad theory of open quantum systems", Phys. Rev. A 75, 022103 (2007).
[EG07] M. Esposito and P. Gaspard, "Quantum master equation for the microcanonical ensemble", Phys. Rev. E 76, 041134 (2007).
[FB07] J. Fischer and H.-P. Breuer, "Correlated projection operator approach to non-markovian dynamics in spin baths", Phys. Rev. A 76, 052119 (2007).
[HKP +07] R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. K. Vandersypen, "Spins in few-electron quantum dots", Rev. Mod. Phys. 79, 1217-1265 (2007).
[ELB10] M. Esposito, K. Lindenberg, and C. V. den Broeck, "Entropy production as correlation between system and reservoir", New J. Phys. 12, 013013 (2010).
[Neu10] J. von Neumann, "Proof of the ergodic theorem and the h-theorem in quantum mechanics", Eur. Phys. J. H 35, 201-237 (2010).
[NC10] M. A. Nielsen and I. L. Chuang, Quantum computation and quantum information: 10th anniversary edition (Cambridge University Press, 2010).
[BMS+12] J.-P. Brantut, J. Meineke, D. Stadler, S. Krinner, and T. Esslinger, "Conduction of ultracold fermions through a mesoscopic channel", Science 337, 1069-1071 (2012).
[LRW+12] N. Li, J. Ren, L. Wang, G. Zhang, P. Hänggi, and B. Li, "Colloquium: phononics: manipulating heat flow with electronic analogs and beyond", Rev. Mod. Phys. 84, 1045-1066 (2012).
[RH12] A. Rivas and S. F. Huelga, Open quantum systems, Vol. 10 (Springer, 2012).
[Wei12] U. Weiss, Quantum dissipative systems, 4th (WORLD SCIENTIFIC, 2012).
[Wil12] F. Wilczek, "Quantum time crystals", Phys. Rev. Lett. 109, 160401 (2012).
[BGM+13] J.-P. Brantut, C. Grenier, J. Meineke, D. Stadler, S. Krinner, C. Kollath, T. Esslinger, and A. Georges, "A thermoelectric heat engine with ultracold atoms", Science 342, 713-715 (2013).
[LL13] L. D. Landau and E. M. Lifshitz, Course of theoretical physics (Elsevier, 2013).
[LSC+13] P. London, J. Scheuer, J.-M. Cai, I. Schwarz, A. Retzker, M. B. Plenio, M. Katagiri, T. Teraji, S. Koizumi, J. Isoya, R. Fischer, L. P. McGuinness, B. Naydenov, and F. Jelezko, "Detecting and polarizing nuclear spins with double resonance on a single electron spin", Phys. Rev. Lett. 111, 067601 (2013).
[Sli13] C. P. Slichter, Principles of magnetic resonance, third edition, Vol. 1 (Springer Science \& Business Media, 2013).
[UMA+13] B. Urbaszek, X. Marie, T. Amand, O. Krebs, P. Voisin, P. Maletinsky, A. Högele, and A. Imamoglu, "Nuclear spin physics in quantum dots: an optical investigation", Rev. Mod. Phys. 85, 79-133 (2013).
[LPK14] A. C. Y. Li, F. Petruccione, and J. Koch, "Perturbative approach to markovian open quantum systems", Sci. Rep. 4, 4887 (2014).
[Sch14] G. Schaller, Open quantum systems far from equilibrium, Vol. 881 (Springer, 2014).
[SLC+14] A. O. Sushkov, I. Lovchinsky, N. Chisholm, R. L. Walsworth, H. Park, and M. D. Lukin, "Magnetic resonance detection of individual proton spins using quantum reporters", Phys. Rev. Lett. 113, 197601 (2014).
[CPF15] M. Campisi, J. Pekola, and R. Fazio, "Nonequilibrium fluctuations in quantum heat engines: theory, example, and possible solid state experiments", N. J. Phys. 17, 035012 (2015).
[FMP15] N. Freitas, E. A. Martinez, and J. P. Paz, "Heat transport through ion crystals", Phys. Scr. 91, 013007 (2015).
[MLS+15] C. Müller, J. Lisenfeld, A. Shnirman, and S. Poletto, "Interacting twolevel defects as sources of fluctuating high-frequency noise in superconducting circuits", Phys. Rev. B 92, 035442 (2015).
[Ven15] L.C.Venuti, "The recurrence time in quantum mechanics", arXiv:1509.04352 (2015).
[BES16] G. Bulnes Cuetara, M. Esposito, and G. Schaller, "Quantum thermodynamics with degenerate eigenstate coherences", Entropy 18, 10 . 3390 /e18120447 (2016).
[HCS+16] D. Halbertal, J. Cuppens, M. B. Shalom, L. Embon, N. Shadmi, Y. Anahory, H. R. Naren, J. Sarkar, A. Uri, Y. Ronen, Y. Myasoedov, L. S. Levitov, E. Joselevich, A. K. Geim, and E. Zeldov, "Nanoscale thermal imaging of dissipation in quantum systems", Nature 539, 407-410 (2016).
[PSG16] J. P. Pekola, S. Suomela, and Y. M. Galperin, "Finite-size bath in qubit thermodynamics", J. Low Temp. Phys. 184, 1015-1029 (2016).
[RR16] C. C. Rusconi and O. Romero-Isart, "Magnetic rigid rotor in the quantum regime: theoretical toolbox", Phys. Rev. B 93, 054427 (2016).
[CCL+17] S. Choi, J. Choi, R. Landig, G. Kucsko, H. Zhou, J. Isoya, F. Jelezko, S. Onoda, H. Sumiya, V. Khemani, C. von Keyserlingk, N. Y. Yao, E. Demler, and M. D. Lukin, "Observation of discrete time-crystalline order in a disordered dipolar many-body system", Nature 543, 221-225 (2017).
[Fra17] F. Franchini, An introduction to integrable techniques for one-dimensional quantum systems, Vol. 940 (Springer, 2017).
[FP17] N. Freitas and J. P. Paz, "Fundamental limits for cooling of linear quantum refrigerators", Phys. Rev. E 95, 012146 (2017).
[SSB+17] P. Strasberg, G. Schaller, T. Brandes, and M. Esposito, "Quantum and information thermodynamics: a unifying framework based on repeated interactions", Phys. Rev. X 7, 021003 (2017).
[VA17] I. de Vega and D. Alonso, "Dynamics of non-markovian open quantum systems", Rev. Mod. Phys. 89, 015001 (2017).
[ZHK+17] J. Zhang, P. W. Hess, A. Kyprianidis, P. Becker, A. Lee, J. Smith, G. Pagano, I. .-D. Potirniche, A. C. Potter, A. Vishwanath, N. Y. Yao, and C. Monroe, "Observation of a discrete time crystal", Nature 543, 217-220 (2017).
[GHU18] Z. Gong, R. Hamazaki, and M. Ueda, "Discrete time-crystalline order in cavity and circuit qed systems", Phys. Rev. Lett. 120, 040404 (2018).
[SST+18] I. Schwartz, J. Scheuer, B. Tratzmiller, S. Müller, Q. Chen, I. Dhand, Z.-Y. Wang, C. Müller, B. Naydenov, F. Jelezko, and M. B. Plenio, "Robust optical polarization of nuclear spin baths using hamiltonian engineering of nitrogen-vacancy center quantum dynamics", Sci. Adv. 4, eaat8978 (2018).
[BCG+19] F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso, Thermodynamics in the quantum regime: fundamental aspects and new directions, Vol. 195 (Springer, 2019).
[Cai19] X. Cai, "Quantum dynamics in a fluctuating environment", Entropy 21, $10.3390 / \mathrm{e} 21111040$ (2019).
[KMS19] V. Khemani, R. Moessner, and S. Sondhi, "A brief history of time crystals", arXiv:1910.10745 (2019).
[MSC19] M. Mehboudi, A. Sanpera, and L. A. Correa, "Thermometry in the quantum regime: recent theoretical progress", J. Phys. A: Math. Theor. 52, 303001 (2019).
[MCL19] C. Müller, J. H. Cole, and J. Lisenfeld, "Towards understanding two-level-systems in amorphous solids: insights from quantum circuits", Rep. Prog. Phys. 82, 124501 (2019).
[RMP+19] A. Riera-Campeny, M. Mehboudi, M. Pons, and A. Sanpera, "Dynamically induced heat rectification in quantum systems", Phys. Rev. E 99, 032126 (2019).
[SDA19a] D. Šafránek, J. M. Deutsch, and A. Aguirre, "Quantum coarse-grained entropy and thermalization in closed systems", Phys. Rev. A 99, 012103 (2019).
[SDA19b] D. Šafránek, J. M. Deutsch, and A. Aguirre, "Quantum coarse-grained entropy and thermodynamics", Phys. Rev. A 99, 010101(R) (2019).
[KBS+20] B. Karimi, F. Brange, P. Samuelsson, and J. P. Pekola, "Reaching the ultimate energy resolution of a quantum detector", Nat. Commun. 11, 367 (2020).
[LP20] G. T. Landi and M. Paternostro, "Irreversible entropy production, from quantum to classical", arXiv:2009.07668 (2020).
[RMS20] A. Riera-Campeny, M. Moreno-Cardoner, and A. Sanpera, "Time crystallinity in open quantum systems", Quantum 4, 270 (2020).
[ŠAS+20] D. Šafránek, A. Aguirre, J. Schindler, and J. Deutsch, "A brief introduction to observational entropy", arXiv:2008.04409 (2020).
[SŠA20] J. Schindler, D. Šafránek, and A. Aguirre, "Entanglement entropy from coarse-graining in pure and mixed multipartite systems", arXiv:2005.05408 (2020).
[HFM + 21] S. Häusler, P. Fabritius, J. Mohan, M. Lebrat, L. Corman, and T. Esslinger, "Interaction-assisted reversal of thermopower with ultracold atoms", Phys. Rev. X 11, 021034 (2021).
[KKG+21] H. Keßler, P. Kongkhambut, C. Georges, L. Mathey, J. G. Cosme, and A. Hemmerich, "Observation of a dissipative time crystal", Phys. Rev. Lett. 127, 043602 (2021).
[LGR+21] M. Lewenstein, A. Gratsea, A. Riera-Campeny, A. Aloy, V. Kasper, and A. Sanpera, "Storage capacity and learning capability of quantum neural networks", Quantum Sci. Technol. 6, 045002 (2021).
[MM21] S. Milz and K. Modi, "Quantum stochastic processes and quantum non-markovian phenomena", PRX Quantum 2, 030201 (2021).
[RSS21a] A. Riera-Campeny, A. Sanpera, and P. Strasberg, "Open quantum systems coupled to finite baths: a hierarchy of master equations", arXiv:2108.01890 (2021).
[RSS21b] A. Riera-Campeny, A. Sanpera, and P. Strasberg, "Quantum systems correlated with a finite bath: nonequilibrium dynamics and thermodynamics", PRX Quantum 2, 010340 (2021).
[Str21] P. Strasberg, (unpublished) quantum stochastic thermodynamics: foundations and selected applications (Oxford University Press, 2021).
[SDR21a] P. Strasberg, M. G. Díaz, and A. Riera-Campeny, "Clausius inequality for finite baths reveals universal efficiency improvements", Phys. Rev. E 104, L022103 (2021).
[SDR21b] P. Strasberg, M. G. Díaz, and A. Riera-Campeny, "Clausius inequality for finite baths reveals universal efficiency improvements", Phys. Rev. E 104, L022103 (2021).
[SW21] P. Strasberg and A. Winter, "First and second law of quantum thermodynamics: a consistent derivation based on a microscopic definition of entropy", PRX Quantum 2, 030202 (2021).
[WKO21] H. Weimer, A. Kshetrimayum, and R. Orús, "Simulation methods for open quantum many-body systems", Rev. Mod. Phys. 93, 015008 (2021).

