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ENERGY CONSERVATION IN OPEN QUANTUM SYSTEMS

master's thesis

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ABSTRACT

The Lindblad theory of open quantum systems has been successfully applied in various fields ranging from quantum optics, condensed matter physics, and quantum thermodynamics to quantum chemistry. Nevertheless, there are situations where we can compare its predictions to those of exact methods or numerically exact results and find discrepancies between them [1]. One example is the case where a single harmonic oscillator is coupled to a thermal bath of independent harmonic oscillators. In this case, for certain parameters, the exact master equation describes equilibration of the system to a thermal state with a temperature different from the one predicted by the Lindblad master equation [2]. The Lindblad theory, based on a weak coupling between the system and environment as well as the Born-Markov approximation, predicts that the system will evolve to a thermal state whose temperature is equal to the initial temperature of the bath. This result is a consequence of the Born approximation, which supposes that throughout the evolution, the bath only fluctuates around its initial equilibrium state.[1] In this master thesis we study the validity of the Born approximation as well as its consistency with other approximations.

By starting from a Hamiltonian for the total system we show that, if the the Born approximation is not invoked, the dynamics of the system is determined by a hierarchy of equations for matrices which can be used to reconstruct the reduced density matrix of the system. This hierarchy approach is fundamentally different from the standard approach, which describes the system dynamics with a weak-coupling master equation, because the hierarchy does not restrict the amount of entanglement possible between the system and the environment. Furthermore, we show how invoking the Born approximation reduces to the usual result and how a generalised ansatz, which we refer to as a generalised Born approximation, reduces the hierarchy to a master equation where the bath temperature is an additional degree of freedom. Finally, we analyse the conservation of the energy of the total system and its relationship to the Markov and secular approximations, and discuss whether imposing it as a condition can fix the time-dependent temperature.

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[1] More specifically, the system and environment become correlated during the evolution, but the latter is continually being projected to its initial state.

CONTENTS

1

INTRODUCTION

A quantum system is called *open* if it is coupled to another quantum system commonly referred to as the environment. The main objective of the study of open quantum systems is to derive effective equations that describe the dynamics of the system while taking into account the most important effects due to its coupling to the environment. Different approaches used to achieve this goal exist, which can be roughly divided into two categories: stochastic and master equation approaches.

1. The master equation approach aims to derive a closed form equation, called a master equation, for the time derivative of the reduced density matrix of the system. In this case the effect of the environment is encoded in the correlation functions of the environment that show up in the master equation.

2. The stochastic approach describes the effect of the system using random variables. These random variables are used to formulate a stochastic version of Schrödinger's equation which includes the effect of the environment as noise variables. Predictions for the evolution of state vectors of the system are then obtained by averaging over many solutions of the stochastic Schrödinger equation.

In many cases there exists a correspondence between master equations and stochastic Schrödinger equations. Stochastic approaches that capture the reduced dynamics of the system are called *unravellings*, of which stochastic Schrödinger equations are a particular example. In cases where this correspondence exists it allows one to tackle the same problem from different angles, throughout this thesis however, we restrict ourselves to the master equation approach.

This chapter is devoted to an exposition of the main concepts in the theory of open quantum systems. We start by formally introducing what we mean by an open quantum system and introduce the model Hamiltonian we consider throughout this thesis in section 1.1. In section 1.2 we motivate the study of open quantum systems from both a fundamental and a practical point of view. Finally, we consider some specific examples for the model Hamiltonian considered and connect them to physical systems that they can be used to describe in section 1.3.

1.1 WHAT IS AN OPEN QUANTUM SYSTEM

As mentioned in the introduction to this chapter, an open quantum system is a quantum system S coupled in some way to another quantum system E called the environment. Usually the Hilbert space dimension of the environment is assumed to be far bigger than the Hilbert space dimension of the system, which validates the use of certain crucial approximations. Assuming that the environment is sufficiently isolated from the rest of the universe we can consider the combined system consisting of S and E as an isolated quantum system.[1] Suppose the Hamiltonian of the system and environment are given by H_S and H_E respectively, then the Hamiltonian of the total system can be written as

$$H = H_S + H_E + H_{SE} \tag{1}$$

where H_{SE} describes the coupling between S and E.

The effective equations of motion for the dynamics of the system S that we aim to derive take the form of differential equations for the reduced density matrix $\rho_S(t)$. The reduced density matrix is the partial trace over the environment of the density matrix of the total system, i.e.

$$\rho_S(t) = \mathrm{Tr}_E\left[\rho_{tot}(t)\right]. \tag{2}$$

At this point we would like to point out that since the size of the reduced density matrix grows quadratically with the Hilbert space dimension of the system, solving a master equation numerically is only feasible if the latter is small enough.

When confronted for the first time with the problem of describing the effective dynamics of a subsystem of a larger isolated quantum system, one might be tempted to think that it is a trivial question. After all, the time evolution of the total system is given by

$$\rho_{tot}(t) = e^{-iH_{tot}t}\rho_{tot}(0)e^{iH_{tot}t}. \tag{3}$$

In principle the evolution of any subsystem of the total system could then be obtained by taking the partial trace over the degrees of freedom we are not interested in. However, this partial trace can only be performed without additional approximations in a few cases. One of the main objectives of the theory of open quantum systems is therefore to find the right approximations using which closed form equations for the reduced density matrix can be derived.

Master equations come in two major varieties, they are either in time-local form or in an integral form:

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[1] In section 1.2 we argue that no quantum system can be considered to be truly isolated from the rest of the universe. However, if we are only interested in the dynamics of S, we can consider the total system consisting of S and E to be modelled as an isolated quantum system if the effect of the rest of the universe on E is negligible for the dynamics of S.

1. Time-local master equations are master equations that can be written as
$$\dot{\rho}_S(t) = \mathcal{L}_t[\rho_S(t)], \tag{4}$$
where $\mathcal{L}_t$ is some operator on the space of density matrices.

2. Master equations in integral form depend in some way on the evolution history of the reduced density matrix. A well-known master equation in integral form is the Nakajima-Zwanzig master equation, which, for factorised initial conditions, can be written as
$$\dot{\rho}_S(t) = \int_{t_0}^{t} \mathcal{K}(t,s)\rho_S(s)ds \tag{5}$$
where $\mathcal{K}$ is some operator that acts on the space of density matrices. If the initial conditions are not factorised, i.e. the system and environment are entangled at the initial time t_0, the Nakajima-Zwanzig master equation also has a contribution from the initial conditions.

Throughout this thesis we will restrict ourselves to time-local master equations of the form whose properties we discuss in section 2.1.

Our discussion thus far does not consider a particular model for the system or environment. Throughout this thesis however, we consider the case where the bath Hamiltonian is a sum of harmonic oscillators and the coupling between the system and the bath is linear. More precisely, the general model Hamiltonian in Eq. (1) is replaced by

$$H = H_S + \sum_{\lambda} \omega_\lambda b_\lambda^\dagger b_\lambda + \sum_{\lambda} g_\lambda (b_\lambda L^\dagger + b_\lambda^\dagger L). \tag{6}$$

Here $b_\lambda^\dagger$ and b_λ are bosonic creation and annihilation operators respectively, whereas L is a system operator and g_λ denotes the coupling between the system and a particular bosonic mode of the environment. This is the most general model Hamiltonian for a system and environment which are coupled in a linear fashion [3].

1.2 WHY STUDY OPEN QUANTUM SYSTEMS

The study of open quantum systems is an inevitable consequence of the fact that, in practice, almost no small quantum system can be considered to be truly isolated from its surroundings. Even in the extreme case of a single hydrogen atom in the near-perfect vacuum between galaxies we need to take into account the environment, in the form of vacuum fluctuations of the electromagnetic field, to explain the Lamb shift of its energy levels. A more down-to-earth example where the theory of open quantum systems is necessary would be an experiment where some small quantum system is probed, using, laser light for example. The number of examples where the theory of open quantum systems can be applied and their diversity is one indicator of the importance of its study.

Apart from its broad applicability, the study of open quantum systems can be considered worthwhile due to its past accomplishments. Most notably, it it has been successful in describing fundamental phenomena such as decoherence and irreversibility in the weak coupling limit. Furthermore, the theory of open quantum systems has provided a theoretical framework for describing experiments for several decades, in particular for those in the field of quantum optics where its study began [4–6]. More recently, the theory of open quantum systems has been used to study the laws of thermodynamics in quantum mechanics [7].

By mentioning the past accomplishments of the theory of open quantum systems we by no means intend to imply its study is primarily of historical value. On the contrary, as the technical prowess of experimentalists evolves, a quantum description for experimental set-ups where quantum systems such as optical cavities and quantum dots interact with their environments become all the more important.

1.3 EXAMPLES OF OPEN QUANTUM SYSTEMS

In this section we discuss three examples of open quantum systems that can be described by the model Hamiltonian we consider throughout this thesis, i.e. the one proposed in Eq. (8). The first example we consider is the Jaynes-Cummings model, which can be used to describe the interaction of a two-level atom with light in an idealised optical cavity. The second model we consider is called the damped Jaynes-Cummings model, which differs from the Jaynes-Cummings model in the sense that the total system consisting of the atom and the cavity is not isolated. Instead, the cavity mode itself is coupled to an an environment of harmonic oscillators as well. Finally we consider the model Hamiltonian for quantum Brownian motion.

The Hamiltonian corresponding to the Jaynes-Cummings model is

$$H = \omega_0 \sigma_+ \sigma_- + \omega b^\dagger b + g_\omega (b\sigma_+ + b^\dagger \sigma_-). \tag{7}$$

Here σ_+ and σ_- are creation and annihilation operators for the two-level system whereas $b^\dagger$ and b are creation and annihilation operators for the cavity mode which is represented by a harmonic oscillator. The interaction term allows the cavity mode and the two-level atom to exchange energy which corresponds to the emission and absorption of photons by the two-level atom.

It is interesting to note that the Jaynes-Cummings model describes a cavity that is ideal in the following sense. It supposes the total system consisting of two-level atom and cavity to be perfectly isolated from its surroundings and it supposes the cavity to accommodate only a single frequency. In practice however, these ideal conditions may not be satisfied, in which case the damped Jaynes-Cummings model might be a more accurate description.

The difference between the Jaynes-Cummings and the damped Jaynes-Cummings model is that in the latter case the cavity mode is coupled to an environment of harmonic oscillators, which we assume to be in their respective ground states. It turns out that provided that there is at most a single quantum in the combined system comprising of two-level atom and the cavity mode, the cavity can be eliminated from the model, i.e. we can consider the two-level atom to be coupled to the environment influencing the cavity directly. In this case the model can be described by the following Hamiltonian

$$H = \omega_0 \sigma_+ \sigma_- + \sum_\lambda \omega_\lambda b_\lambda^\dagger b_\lambda + \sum_\lambda g_\lambda (b_\lambda \sigma_+ + b_\lambda^\dagger \sigma_-), \tag{8}$$

provided that the coupling constants g_λ are chosen in such a way that the dynamics of the two-level atom resembles that of an identical two-level atom coupled to a continuous bath of harmonic oscillators whose spectral density is a Lorentzian given by [8]

$$J(\omega) = \frac{1}{2\pi} \frac{\eta W}{(\omega - \omega_0)^2 + W^2}. \tag{9}$$

Here η denotes the coupling strength, W determines the width of the Lorentzian, and ω_0 is the frequency of the two-level system. This simulation of a continuous environment by a finite set of harmonic oscillators is a recurring theme in the field which we return to in section 4.2.3.

The final model we consider in this thesis is that of quantum Brownian motion, which refers to systems described by Hamiltonians of the form

$$H = \omega_0 a^\dagger a + \sum_\lambda \omega_\lambda b_\lambda^\dagger b_\lambda + \sum_\lambda g_\lambda (b_\lambda a^\dagger + b_\lambda^\dagger a). \tag{10}$$

Thus instead of a two-level system the open system under consideration is described by a harmonic oscillator.

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THE LINDBLAD THEORY OF OPEN QUANTUM SYSTEMS

In this chapter we review some basic aspects of the theory of open quantum systems focusing on time-local master equations in Lindblad form. Time-local master equations in Lindblad form arise naturally when imposing a number of physical constraints on the effective equations describing the dynamics of an open quantum system. They provide a framework for describing irreversible dynamics of quantum systems coupled to larger environments. In particular, this framework can be used to describe equilibration as well as thermalisation and is consistent with the second law of thermodynamics. These features, amongst other things, explain why master equations in Lindblad form have found applications in areas as diverse as quantum optics, condensed matter physics and ultra-cold quantum gasses. Although at the end of this chapter we argue that in certain cases the approach usually taken to obtain equations of the Lindblad type, which comes down to imposing the Born-Markov approximation, can no longer be justified, many of the arguments in this chapter still apply to the generalised formalism we propose in chapter 3.

The structure of this chapter is as follows. In section 2.1 we consider what conditions the reduced dynamics should satisfy and what implications this has for the form of the equations. Then we discuss how requiring a semi-group property leads to the well-known Lindblad form of the master equation in section 2.2. In section 2.3 we derive a master equation in Lindblad form from the model Hamiltonian introduced in section 1.1. Following this, we review some of the properties of this master equation in Lindblad form regarding equilibration, thermalisation and the second law of thermodynamics in section 2.4. In the final sections of this chapter we discuss some of the deficiencies of master equations in Lindblad form and consider a particular generalisation of the Lindblad theory of open quantum systems.

2.1 TIME-LOCAL MASTER EQUATIONS

As explained in chapter 1 the theory of open quantum systems concerns itself with effective equations that describe a quantum mechanical system coupled to an environment whose Hilbert space is large compared to that of the system. In this thesis we restrict ourselves to time-local master equations which is why we review what restrictions certain commonly imposed physical requirements on time-local master equations lead to. For a more detailed overview of properties of time-local master equations we refer the reader to appendix A of [9], on which we based this section, and references therein.

Recall that time-local master equations are evolution equations for the reduced density matrix of the form

$$\dot{\rho}_S(t) = \mathcal{L}_t[\rho_S(t)], \tag{11}$$

with $\mathcal{L}_t$ a linear operator acting on the space of density matrices, called a *generator*. It turns out that such an equation can always be written as

$$\mathcal{L}_t[\rho_S] = \sum_k A_k(t)\rho_S(t)B_k^\dagger(t). \tag{12}$$

with A_k and B_k time-dependent operators acting on states in the Hilbert space of the system. For such an evolution equation to represent a physical process it should preserve certain properties of the reduced density matrix throughout its evolution such as its hermiticity and trace.

In the case where the Hilbert space of the system is finite dimensional, it can be proven constructively that imposing hermiticity and preservation of the trace implies that Eq. (12) can be written as

$$\dot{\rho}_S(t) = -\frac{i}{\hbar}[H, \rho_S(t)] + \sum_{i,j=1}^{N-1} d_{ij}(t)\left(G_i\rho_S(t)G_j - \frac{1}{2}[G_jG_i, \rho_S(t)]\right) \tag{13}$$

with G_i a particular basis of the finite-dimensional state space of the system, $d_{ij}(t)$ entries of what is called the decoherence matrix, and H a hermitian operator often referred to as the Lamb shift Hamiltonian. The properties the basis G_i has to satisfy as well as expressions for d_{ij} and H in terms of A_k, B_k and G_i can be found in [9].

An additional requirement the reduced density matrix should continue to satisfy is positivity, i.e. positivity of its eigenvalues. After all, we interpret the eigenvalues of the reduced density matrix as probabilities which should never take on negative values. However, usually a condition stronger than positivity called complete positivity is imposed, which amounts to requiring the density matrix of which ρ_S is the partial trace to be positive. The dynamics described by a master equation of the form described in Eq. (13) is completely positive if the elements $d_{ij}(t)$ of the decoherence matrix are positive at all times.

2.2 MASTER EQUATIONS IN LINDBLAD FORM

In section 2.1 we discussed what restrictions requiring basic physical properties such as preservation of the trace, hermiticity and complete positivity of the reduced density matrix imposes on the form that a time-local master equation can take. An additional property that is often satisfied by the dynamics of the system is that its dynamics is irreversible. Although true irreversibility is only possible if the

Hilbert space dimension of the environment diverges, i.e. the environment is continuous, we often take the dynamics to be irreversible if the environment is large enough so that reversible effects can be neglected. One requirement that is often satisfied in such cases is that an operator called the *evolution operator*, which we define below, satisfies a condition that is called the *semi-group property*. If this semigroup property is satisfied, the mathematical theory is particularly well-developed, although in recent years the field has increasingly focused on extensions of the theory that do not impose this assumption.

The evolution operator is the operator that evolves $\rho_S(t)$ through time, i.e. it is the operator such that

$$\rho_S(t+s) = \Lambda_t[\rho_S(s)] \tag{14}$$

The semigroup property of the evolution operator Λ_t, which is a statement of irreversibility, is then defined as

$$\Lambda_t \Lambda_s = \Lambda_{t+s} \tag{15}$$

for all t for which Λ_t is defined and all $s \in \mathbb{R}_{>0}$.[1] In other words, using the evolution operator we can always see what a given state evolves to over time, but we can not see what state it might have been at an earlier time. This is the sense in which we mean that the reduced dynamics of the system is irreversible.

Recall the particular form the master equation was forced to take after imposing preservation of the trace and hermiticity as described in Eq. (13). Such a master equation, where we do not yet make any claims about positivity of the elements of the decoherence matrix, we will refer to as a Lindblad-type master equation.

It has been shown by Lindblad [10] and under slightly different conditions by Gorini, Kossakowski, and Sudarshan [11] that if the evolution operator Λ_t satisfies the semigroup property in addition to the requirements that led to Eq. (13) and preserves complete positivity the master equation can be written as a Lindblad-type equation with constant positive decoherence matrix. In fact, the converse statement is also true, i.e. if a master equation can be written as a Lindblad-type master equation with time-independent positive decoherence matrix the dynamics it describes preserves complete positivity and satisfies a semi-group property. Such master equations with time-independent positive decoherence matrix we refer to as master equations in Lindblad form.

2.3 DERIVING A MASTER EQUATION IN LINBLAD FORM

In the previous sections we have shown how the form a time-local master equation can take is restricted by imposing certain physical

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[1] Of course Λ_{t+s} should be defined for all combinations of t and s so we assume that Λ_t is defined for all $t \in [t_0, \infty)$ for some $t_0 \in \mathbb{R}$.

conditions. However, thus far we have not yet shown how such a master equation can be derived from a Hamiltonian for the total system comprising of system and environment. In this section we derive a time-local master equation in Lindblad form for the model Hamiltonian introduced in section 1.1.

Starting from the total system we know that the time evolution for the total density matrix in the interaction picture is given by

$$\dot{\rho}(t) = [H_I(t), \rho(t)] \tag{16}$$

where $H_I(t)$ is the interaction picture Hamiltonian and $\rho(t)$ is the density matrix in the interaction picture. A formal solution can be obtained from Eq. (16) by integrating w.r.t. time, which gives

$$\rho(t) = \rho(t_0) + \int_{t_0}^{t} ds [H_I(s), \rho(s)]. \tag{17}$$

Substituting back the solution into the evolution equation for the reduced density matrix we find

$$\dot{\rho}(t) = [H_I(t), \rho(t_0)] + \int_{t_0}^{t} ds [H_I(t), [H_I(s), \rho(s)]]. \tag{18}$$

An evolution equation for the reduced density matrix is then obtained by taking the partial trace over the environmental degrees of freedom

$$\dot{\rho}_S(t) = \mathrm{Tr}_E \left\{ [H_I(t), \rho(t_0)] + \int_{t_0}^{t} ds [H_I(t), [H_I(s), \rho(s)]] \right\}. \tag{19}$$

Although this is an evolution equation for the reduced density matrix from the initial Hamiltonian obtained without doing any approximations, it is of limited use. After all, if one would want to use it to do numerics without additional simplifications, the total density matrix would have to be used, which is a huge object if the Hilbert space dimension of the bath is large. Therefore we now show how this equation can be further simplified under certain assumptions until we have a time-local master equation in Lindblad form.

Suppose the spectrum of H_S is discrete, then the system operators can be decomposed as

$$L(t) = \sum_{\omega} e^{-i\omega t} L(\omega) \tag{20}$$

$$L^{\dagger}(t) = \sum_{\omega} e^{i\omega t} L^{\dagger}(\omega) \tag{21}$$

where

$$L(\omega) = \sum_{\epsilon' - \epsilon = \omega} \Pi(\epsilon)\, L\, \Pi(\epsilon'). \tag{22}$$

Here $\Pi(\epsilon)$ denotes a projection operator onto the eigenspace of H_S corresponding to the eigenvalue ϵ. Plugging the expansion in Eq. (20)

and Eq. (21) into Eq. (19) gives rise to terms containing the phase factor

$$e^{\pm i(\omega-\omega')t} \tag{23}$$

where ω and ω' are the expansion parameters. If the typical time scale for the evolution of the system is large compared to $|\omega-\omega'|^{-1}$, the oscillations average out over time allowing us to neglect them unless $\omega=\omega'$. This approximation is called the rotating wave approximation in quantum optics or the secular approximation.

Replacing $\rho(s)$ by $\rho(t)$ in Eq. (19), which is valid up to second order in perturbation theory, as well as assuming the secular approximation to hold, Eq. (19) reduces to

$$\begin{aligned}\dot{\rho}_S(t) = \operatorname{Tr}&\left[\left(\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}(L^\dagger(\omega)\rho_S(t)L(\omega)\otimes b_\lambda\rho_B b_\lambda^\dagger)\right)\right]\\ -\operatorname{Tr}&\left[\left(\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}(L(\omega)L^\dagger(\omega)\rho_S(t)\otimes b_\lambda^\dagger b_\lambda\rho_B)\right)\right]\\ +\operatorname{Tr}&\left[\left(\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}(L(\omega)\rho_S(t)L^\dagger(\omega)\otimes b_\lambda^\dagger\rho_B b_\lambda)\right)\right]\\ -\operatorname{Tr}&\left[\left(\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}(\rho_S(t)L^\dagger(\omega)L(\omega)\otimes \rho_B b_\lambda b_\lambda^\dagger)\right)\right]\\ +\text{h.c.}&+\sum_\lambda O(g_\lambda^4)\end{aligned} \tag{24}$$

where

$$\rho_B = \frac{e^{-\beta H_B}}{\operatorname{Tr}_B\left[e^{-\beta H_B}\right]}. \tag{25}$$

Performing the partial trace of this equation gives

$$\begin{aligned}\dot{\rho}_S(t) = &\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}L^\dagger(\omega)\rho_S(t)L(\omega)\overline{n}_\lambda(\beta)\\ &-\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}L(\omega)L^\dagger(\omega)\rho_S(t)\overline{n}_\lambda(\beta)\\ &+\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}L(\omega)\rho_S(t)L^\dagger(\omega)(\overline{n}_\lambda(\beta)+1)\\ &-\sum_{\omega,\lambda}\int_0^t ds g_\lambda^2 e^{i(\omega_\lambda-\omega)s}\rho_S(t)L^\dagger(\omega)L(\omega)(\overline{n}_\lambda(\beta)+1)\\ &+\text{h.c.}+\sum_\lambda O(g_\lambda^4)\end{aligned} \tag{26}$$

where

$$\overline{n}_\lambda(\beta) := \frac{1}{e^{\beta\omega_\lambda}-1}. \tag{27}$$

One can check that this equation is in Lindblad-like form with $d_{ij}(t) \propto \delta_{ij}$ due to the secular approximation we did earlier. The explicit time-dependence of the pre-factors however, indicates that we have not yet arrived at an equation in Lindblad form.

To rid the elements of the decoherence matrix of their time-dependence, a final approximation is required. Supposing that

$$\sum_\lambda g_\lambda^2 e^{i(\omega_\lambda-\omega)s} \tag{28}$$

drops off sufficiently fast, we can let the upper bound of the integral go to infinity without introducing a large error.[2] Furthermore, it implicitly assumes that after it has decayed there is no revival, which is equivalent to saying that the Hilbert space dimension of the bath diverges. Therefore we should be able to describe the sum over λ's with an integral, i.e. there should be a function $J(\tilde{\omega})$ such that

$$\sum_\lambda g_\lambda^2 = \int d\tilde{\omega} J(\tilde{\omega}). \tag{29}$$

Now we can use

$$\int_0^\infty e^{\pm i\omega t'} dt' = \pm i\mathcal{P}\frac{1}{\omega} + \pi\delta(\omega), \tag{30}$$

to obtain

$$\begin{aligned}
\dot{\rho}_S(t) = &- i[H_{LS}, \rho_S(t)] \\
&- \pi \sum_\omega J(\omega)\overline{n}(\beta,\omega) \left\{ L(\omega)L^\dagger(\omega), \rho_S(t) \right\} \\
&- \pi \sum_\omega J(\omega)(\overline{n}(\beta,\omega)+1) \left\{ L^\dagger(\omega)L(\omega), \rho_S(t) \right\} \\
&+ 2\pi \sum_\omega J(\omega)(\overline{n}(\beta,\omega)+1)L(\omega)\rho_S(t)L^\dagger(\omega) \\
&+ 2\pi \sum_\omega J(\omega)\overline{n}(\beta,\omega)L^\dagger(\omega)\rho_S(t)L(\omega) \\
&+ \sum_\lambda O(g_\lambda^4).
\end{aligned} \tag{31}$$

where

$$\begin{aligned}
H_{LS} = &\sum_\omega \mathcal{P} \int_0^\infty d\tilde{\omega} \frac{J(\tilde{\omega})}{\tilde{\omega}-\omega} \overline{n}(\beta,\tilde{\omega}) L(\omega)L^\dagger(\omega) \\
&+ \sum_\omega \mathcal{P} \int_0^\infty d\tilde{\omega} \frac{J(\tilde{\omega})}{\tilde{\omega}-\omega} (\overline{n}(\beta,\tilde{\omega})+1) L^\dagger(\omega)L(\omega)
\end{aligned} \tag{32}$$

is called the Lamb shift Hamiltonian. Note that we have achieved our goal of deriving a master equation in Lindblad form from first principles. For some purposes however, it can also be useful to write this master equation in a different form which we describe next.

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[2] A bath that satisfies these requirements is called Markovian, which reflects the independence of the time evolution from its evolution history.

If the spectrum of the system Hamiltonian is discrete, we can expand ρ in an energy eigenbasis giving

$$\rho_S = \sum_k p_k |\psi_k\rangle\langle\psi_k| \tag{33}$$

with p_k the population of a given energy state. In this case an evolution equation for the populations can be obtained from Eq. (31) by wedging both the left and right hand side with an energy eigenstate. This gives

$$\dot{p}_m(t) = \sum_{m'} W_{mm'} p_{m'}(t) \tag{34}$$

with

$$W_{mm'} = \begin{cases} A_{mm'} & \text{if } m \neq m' \\ -\sum_{n\neq m'} A_{nm'} & \text{if } m = m' \end{cases} \tag{35}$$

where we defined

$$\begin{aligned} A_{mm'} =& -2\pi J(\epsilon_{m'}-\epsilon_m)\overline{n}(\beta,\epsilon_{m'}-\epsilon_m)\langle\psi_m|L|\psi_{m'}\rangle\langle\psi_{m'}|L^\dagger|\psi_m\rangle \\ & -2\pi J(\epsilon_m-\epsilon_{m'})(\overline{n}(\beta,\epsilon_m-\epsilon_{m'})+1)\langle\psi_m|L^\dagger|\psi_{m'}\rangle\langle\psi_{m'}|L|\psi_m\rangle \end{aligned}$$

Eq. (34) is also referred to as a Pauli rate equation.

The derivation in this section shows how under certain approximations effective equations for the system that take into account the influence of the environment up to leading order in perturbation theory can be derived. We would like to emphasise that here the effect of the environment is incorporated in the master equation via the spectral density and the bath correlation functions.

2.4 ENTROPY PRODUCTION, EQUILIBRATION, AND THERMALISATION

In the macroscopic world we know that a finite system coupled to a heat bath at temperature T approaches a thermal state with the same temperature T.[3] Since this macroscopic behaviour should somehow be the effective behaviour of the underlying quantum description of both system and heat bath, we might hope that master equations in Lindblad form as discussed in section 2.2 predict this behaviour. In this section we give an overview of the predictions of the Lindblad theory of open quantum systems regarding entropy production, equilibration, and thermalisation. The part about entropy production in this section is based on [12] and references therein.

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[3] By heat bath in this situation we mean a system whose heat capacity diverges. Otherwise, the temperature not changing would be inconsistent with energy conservation of the total system.

It is always true that a thermal state for the system at the same temperature as the bath is a steady state solution of Eq. (31). To show this, we plug in

$$\rho_S^{\text{th}} = \frac{e^{-\beta H_S}}{\text{Tr}_S\left[e^{-\beta H_S}\right]}. \tag{36}$$

as an ansatz for $\rho_S(t)$. Using the fact that

$$\rho_S^{th} L(\omega) = e^{\beta\omega} L(\omega) \rho_S^{th} \tag{37}$$

$$\rho_S^{th} L^{\dagger}(\omega) = e^{-\beta\omega} L^{\dagger}(\omega) \rho_S^{th} \tag{38}$$

as a result of the definition for $L(\omega)$, we immediately see that

$$\left[\rho_S^{\text{th}}, H_{LS}\right] = 0 \tag{39}$$

The remaining terms contain factors of the form

$$\left\{L(\omega)L^{\dagger}(\omega), \rho_S^{\text{th}}\right\} = e^{\beta\omega} L(\omega) \rho_S^{\text{th}} L^{\dagger}(\omega) \tag{40}$$

$$\left\{L^{\dagger}(\omega)L(\omega), \rho_S^{\text{th}}\right\} = e^{-\beta\omega} L^{\dagger}(\omega) \rho_S^{\text{th}} L(\omega) \tag{41}$$

From Eq. (40) and Eq. (41) we conclude that our thermal state ansatz is a solution since

$$\overline{n}(\beta, \omega) = (\overline{n}(\beta, \omega) + 1) e^{-\beta' \omega} \tag{42}$$

This shows that the thermal state of the system is indeed a steady state solution of Eq. (31). However, it does not yet prove that this state is always approached in the long time limit. To be able to say more about the steady state that is approached in the long time limit, we consider the entropy of the system.

A quantity intrinsically linked to irreversibility is the entropy, which for a quantum system can be formulated as

$$S(\rho) = -\text{Tr}\left[\rho \ln \rho\right]. \tag{43}$$

Supposing the spectrum of the system Hamiltonian to be discrete, the reduced density matrix can be expanded as in Eq. (33). In this case the equation for the entropy of the system reduces to

$$S(\rho_S) = -\sum_k p_k \ln p_k \tag{44}$$

If we suppose the evolution equation for the p_k to be of the form as described in Eq. (34) with

$$\sum_m W_{mm'} = 0 \tag{45}$$

where now also the W may be time-dependent via some control variable[4], the change in the system's entropy has two contributions. The first comes from the entropy production of the system itself, i.e. the internal entropy production $\dot{S}_i(t)$. The second contribution comes from the entropy change due to the interaction with the environment $\dot{S}_e(t)$. It has been shown that $S_i(t) \geq 0$ at all times and the equality holds if and only if the detailed balance condition is satisfied, i.e. if $\mathcal{L}(\rho) = 0$ where $\mathcal{L}$ is the generator of the master equation under consideration [12, 13].

The conclusion we can draw from this is that unless the system is in a stationary state, the entropy is increasing. Now if the thermal state of the system, which we showed to be a stationary state, is the only stationary state we may conclude that thermal equilibrium is approached regardless of the initial conditions. This is the case if $\mathcal{L}$ has only one eigenvalue whose real part is zero. If this is not the case there may be more stationary states and the stationary state approached in the long time limit may depend on the initial conditions.

2.5 DEFICIENCIES OF MASTER EQUATIONS IN LINDBLAD FORM

One obvious short-coming of Eq. (31) is that certain environments cannot be considered to be Markovian rendering the derivation invalid. This is reflected in the fact that the upper bound of the integral in Eq. (26) cannot be taken to infinity up to the accuracy desired. The obvious work-around however, is to use Eq. (26) as the master equation so that the time-dependence of the coefficients is still respected. Although the preservation of complete positivity is no longer guaranteed by this master equation, it can still be used provided that we work in the weak coupling limit. More can be said about how the theory can be adjusted to describe non-Markovian environments, but this is beyond the scope of this thesis.

A more subtle short-coming concerns energy conservation of the total system. The prediction of the master equation in Lindblad form in Eq. (31) that if the Lindblad generator has a single eigenvalue whose real part is zero, a thermal state is approached whose temperature does not depend on the initial conditions violates energy conservation. After all, if we start in a highly excited state, the system loses energy to the environment as time evolves. Due to the Born approximation however, the bath is not allowed to change so that energy conservation is violated more and more the further away from equilibrium the initial state of the system is taken. In section 3.8 we revisit this inconsistency.

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[4] Actually in chapter 3 we use the result discussed here where the time-dependence comes from the bath temperature. This is not a control variable in the usual sense, but the proof in [12] does not seem to depend on this.

Finally, we note that Eq. (31) is only true if the coupling is sufficiently weak because we neglect the higher order terms in the coupling constant. Also, when the coupling of a quantum system to the environment is strong enough it is expected that the correlations between the system and environment become more important. In this case the assumption that the total system state is a product state is incorrect. In section 3.2 we derive a system of equations that is perturbative, but which can take into account strong correlations between the system and the environment. To be able to compare this result to an already known generalisation of the Lindblad theory proposed by Breuer [14], we devote the next section to his proposal.

2.6 MASTER EQUATIONS IN GENERALISED LINDBLAD FORM

In the previous section we mentioned that one of the short-comings of the master equation in section 2.3 is that it assumes the reduced density matrix to be in a product state throughout its evolution. Although this does not mean that no system-bath correlations are taken into account, as we will see explicitly in section 3.2, it does restrict the effect the correlations between system and bath can have. In this section we discuss a generalisation of the Lindblad theory of open quantum systems as proposed in [14], which allows for a description of open quantum systems that are strongly entangled with their environment.

The main idea is to suppose that the environment can be in a finite number of normalised states, labelled by i, i.e.

$$\rho = \sum_i \rho_i \otimes |i\rangle\langle i|. \tag{46}$$

This extension of the space that the total density matrix is an element of allows for more of the entanglement between the system and environment to be taken into account. The reduced density matrix is obtained from Eq. (46) by taking the partial trace, i.e.

$$\rho_S(t) = \sum_i \rho_i(t). \tag{47}$$

The $\rho_i(t)$ are therefore non-normalised matrices.

Supposing the dynamical map Λ to be completely positive and trace preserving and the initial conditions to be a product state, it can be shown that the evolution equation for ρ_i can be written as

$$\dot{\rho}_i = \mathcal{K}_i^t(\rho_1, \ldots, \rho_n) \tag{48}$$

where the $\mathcal{K}_i^t$ are in general time-dependent but we suppose them to be constant in the following.

A Lindblad generator on the extended space is said to exist if we can write

$$\mathcal{L}\left(\sum_i \rho_i \otimes |i\rangle\langle i|\right) = \mathcal{K}(\rho_1, \ldots, \rho_n) \otimes |i\rangle\langle i| \tag{49}$$

The dynamics is guaranteed to preserve complete positivity as it does for a master equation in Lindblad form. It turns out that such a Lindblad generator exists if and only if the generators $\mathcal{K}_i$ are of the form

$$\mathcal{K}_i(\rho_1, \ldots, \rho_n) = -i[H^i, \rho_i] + \sum_{j\lambda} \left(R_\lambda^{ij} \rho_j R_\lambda^{ij\dagger} - \frac{1}{2} \{ R_\lambda^{ij\dagger} R_\lambda^{ji}, \rho_i \} \right) \tag{50}$$

as shown by Breuer [14]. This is the generalisation of the result proven by Lindblad to an extended space for the total density matrix.

However, it is again not necessary for the generators $\mathcal{K}_i$ to be constant in order to preserve complete positivity. It is also sufficient for the generators to be of the form as described in Eq. (50) with all $H^i(t)$ and $R_\lambda^{ij}(t)$ positive at all times.

3

GENERALISING THE BORN APPROXIMATION

In this chapter we study the Born approximation by attempting to derive a master equation for a particular model without assuming the Born approximation. The model we consider is that of an arbitrary quantum system with a discrete spectrum coupled linearly to an environment of harmonic oscillators introduced in section 1.1. It turns out that if we do not invoke the Born approximation at all, we do not obtain a time-local master equation as usual. Instead, we obtain a coupled system of differential equations for matrices whose sum is equal to the reduced density matrix. Although these equations in principle allow for a treatment of open quantum systems beyond the Born approximation, they are difficult to use in practice. In particular, their numerical implementation is troublesome because the number of equations grows quickly with the number of oscillators in the environment. In order to obtain a set of equations which can be implemented more efficiently, we impose a generalised Born approximation which amounts to assuming the bath remains in a thermal state at all times, albeit with a time-dependent temperature. This assumption is weaker than invoking the Born approximation and results in a master equation for the reduced density matrix by summing over the system of equations derived before. Since we have introduced an additional degree of freedom by allowing the bath temperature to be time-dependent, we have to come up with an additonal constraint. We consider several possible candidates for this constraint and discuss their suitability.

3.1 DERIVING THE SCALAR HIERARCHY

In this section we derive a coupled system of equations determining the time evolution of the entries of the reduced density matrix. This system of equations, whose derivation does not involve any approximations, is one of the basic ingredients of the derivations to follow.

Consider a composite quantum system composed of an arbitrary quantum system S and an environment E consisting of a finite number M of harmonic oscillators. The systems S and E are supposed to be coupled in a linear fashion so that the Hamiltonian of the system can be written in the following form:

$$H = H_S + \sum_{\lambda} \omega_\lambda b_\lambda^\dagger b_\lambda + \sum_{\lambda} g_\lambda (b_\lambda L^\dagger + b_\lambda^\dagger L). \tag{51}$$

Here H_S is the Hamiltonian of the quantum system S, the ω_λ are the oscillator frequencies, and the g_λ are the coupling constants corresponding to the different oscillators.

The quantity for which we want to derive an evolution equation is the reduced density matrix of the system S. To this end, we first consider the total system state $|\Psi(t)\rangle$. Expanding the system part of the total state in an orthogonal basis of energy eigenstates $\{|\psi_r\rangle\}$ and the bath in the occupation number basis $\{|\mathbf{n}\rangle\}$ we get

$$|\Psi(t)\rangle = \left(\sum_r a_r(t)|\psi_r\rangle\right) \otimes \left(\sum_{\mathbf{n}} c_{r,\mathbf{n}}(t)|\mathbf{n}\rangle\right), \tag{52}$$

with

$$\mathbf{n} = (n_1, \ldots, n_M) \in \mathbb{N}_0^M. \tag{53}$$

Each of the M entries refers to the occupation number of the respective oscillator. For notational convenience we write

$$|\Psi(t)\rangle = \sum_{r,\mathbf{n}} a_{r,\mathbf{n}}(t)|\psi_r, \mathbf{n}\rangle, \tag{54}$$

where we used the convention that

$$a_{r,\mathbf{n}}(t) := a_r(t)c_{r,\mathbf{n}}(t). \tag{55}$$

The complex function defined in Eq. (55) is a product of the probability amplitudes of the system S being in an energy eigenstate labelled by r and the environment being in an occupation number basis state described by the vector $\mathbf{n}$.

The reduced density matrix, which is the partial trace of the total density matrix, can then be written as

$$\rho_S(t) = \sum_{\mathbf{n},r,s} a_{r,\mathbf{n}}(t)a^*_{s,\mathbf{n}}(t)|\psi_r\rangle\langle\psi_s| = \sum_{\mathbf{n}} \rho_{\mathbf{n}}(t). \tag{56}$$

Here we defined

$$\rho_{\mathbf{n}}(t) = \sum_{r,s} a_{r,\mathbf{n}}(t)a^*_{s,\mathbf{n}}(t)|\psi_r\rangle\langle\psi_s|, \tag{57}$$

which can be interpreted as a non-normalised matrix describing the subsystem S provided that the environment is in a fixed state $\mathbf{n}$.

In order to compute the time evolution of the coefficients of the matrices defined in Eq. (57), we first consider the Schrödinger equation for the total system in the interaction picture with respect to everything but the coupling terms in the Hamiltonian, which reads

$$\begin{aligned} i\frac{d}{dt}|\Psi(t)\rangle = &\sum_\lambda g_\lambda e^{i\omega_\lambda t} \sum_{v,\mathbf{m}} a_{v,\mathbf{m}}(t)L(t)b^\dagger_\lambda|\psi_v, \mathbf{m}\rangle \\ &+ \sum_\lambda g_\lambda e^{-i\omega_\lambda t} \sum_{v,\mathbf{m}} a_{v,\mathbf{m}}(t)L^\dagger(t)b_\lambda|\psi_v, \mathbf{m}\rangle. \end{aligned} \tag{58}$$

Here $L(t)$ denotes the operator L in the interaction picture, which is given by

$$L(t) := e^{iH_S t} L e^{-iH_S t}. \tag{59}$$

An equation for the time derivative of $a_{r,\mathbf{n}}(t)$ is obtained by applying $\langle \mathbf{n}, \psi_r|$ to both sides of Eq. (58), which gives

$$\begin{aligned} i\dot{a}_{r,\mathbf{n}}(t) = & \sum_{\lambda,v} \sqrt{n_\lambda} g_\lambda e^{i\omega_\lambda t} D_{rv}(t) a_{v,\mathbf{n}-\mathbf{e}_\lambda}(t) \\ & + \sum_{\lambda,v} \sqrt{n_\lambda + 1} g_\lambda e^{-i\omega_\lambda t} U_{r,v}(t) a_{v,\mathbf{n}+\mathbf{e}_\lambda}(t). \end{aligned} \tag{60}$$

Here $\mathbf{e}_\lambda$ denotes the λ^{th} unit vector in $\mathbb{R}^M$ and we defined

$$D_{r,v}(t) := \langle \psi_v | L(t) | \psi_v \rangle, \tag{61}$$

$$U_{r,v}(t) := \langle \psi_r | L^\dagger(t) | \psi_v \rangle, \tag{62}$$

for notational convenience.

The coupled system of differential equations determining the $a_{r,\mathbf{n}}(t)$, i.e. the probability amplitudes for a given configuration, will henceforth be referred to as the *scalar hierarchy*. The first and second term on the right hand side of Eq. (60) can be interpreted as the terms contributing to the flow of quanta of energy from the system to the environment and the other way around respectively. We emphasise that the scalar hierarchy consists of infinitely many equations since we have an equation like Eq. (60), i.e. a *layer* of the hierarchy, for each $\mathbf{n}$ whose entries are non-negative integers. The layers of the scalar hierarchy form the basic building blocks in the derivation of a time evolution equation for the matrices $\rho_{\mathbf{n}}(t)$ in the following sections.

3.2 THE WEAK COUPLING LIMIT

In this section, we will use the scalar hierarchy to derive a system of coupled differential equations for the matrices $\rho_{\mathbf{n}}$. To derive this set of equations for the $\rho_{\mathbf{n}}$ we are forced to do some approximations. In particular, we invoke a weak coupling assumption from now on, i.e. we suppose $g_\lambda^2 \ll g_\mu$ to hold for all λ and μ. Furthermore, we assume that the total state of the system at some initial time t_0, which we take to be 0, is a product state.

To obtain a system of coupled differential equations for the $\rho_{\mathbf{n}}$, we first consider the evolution equations for their coefficients, which we rename to be

$$\rho_{r,\mathbf{n},s,\mathbf{n}}(t) = a_{r,\mathbf{n}}(t) a^*_{s,\mathbf{n}}(t). \tag{63}$$

The time derivative of $\rho_{r,\mathbf{n},s,\mathbf{n}}(t)$, which encodes the time dependence of $\rho_{\mathbf{n}}$, can then be written as

$$\begin{aligned} i\dot{\rho}_{r,\mathbf{n},s,\mathbf{n}}(t) = & \sum_{\lambda,v}\sqrt{n_{1\lambda}}g_\lambda e^{i\omega_\lambda t}D_{r,v}(t)\rho_{v,\mathbf{n}-\mathbf{e}_\lambda,s,\mathbf{n}}(t) \\ & - \sum_{\lambda,w}\sqrt{n_{1\lambda}}g_\lambda e^{-i\omega_\lambda t}U_{w,s}(t)\rho_{r,\mathbf{n},w,\mathbf{n}-\mathbf{e}_\lambda}(t) \\ & + \sum_{\lambda,v}\sqrt{n_{1\lambda}+1}g_\lambda e^{-i\omega_\lambda t}U_{r,v}(t)\rho_{v,\mathbf{n}+\mathbf{e}_\lambda,s,\mathbf{n}}(t) \\ & - \sum_{\lambda,w}\sqrt{n_{1\lambda}+1}g_\lambda e^{i\omega_\lambda t}D_{w,s}(t)\rho_{r,\mathbf{n},w,\mathbf{n}+\mathbf{e}_\lambda}(t) \end{aligned} \tag{64}$$

using Eq. (60).

To obtain a closed form equation for $\rho_{\mathbf{n}}(t)$ from Eq. (64), the right hand side has to be made diagonal in $\mathbf{n}$. This can be achieved by integrating Eq. (64) and plugging it back into itself. The result has terms diagonal in $\mathbf{n}$ as well as terms for which the sum over the indices of the difference of the two vector indices is two. The terms depending on the initial conditions vanish due to the assumption that the initial state is a product state. It is important to note that this is the first and only time that we use this assumption. Furthermore, we want to make explicit that we do not assume the environment to be in a thermal state initially. The terms in the resulting expression that are still non-diagonal in $\mathbf{n}$ can be removed perturbatively by repeatedly substituting the solution to Eq. (60) and keeping only the diagonal terms. Using this procedure of integration and substitution, the time derivative of $\rho_{\mathbf{n}}(t)$ up to quadratic order in the coupling parameters is given by

$$\begin{aligned} \dot{\rho}_{\mathbf{n}}(t) = & -\int_0^t dt' \sum_\lambda g_\lambda^2 e^{i\omega_\lambda(t-t')} n_{1,\lambda} L(t)L^\dagger(t')\rho_{\mathbf{n}}(t') \\ & - \int_0^t dt' \sum_\lambda g_\lambda^2 e^{i\omega_\lambda(t-t')}(n_{1,\lambda}+1)\rho_{\mathbf{n}}(t')L^\dagger(t')L(t) \\ & + \int_0^t dt' \sum_\lambda g_\lambda^2 e^{i\omega_\lambda(t-t')} n_{1,\lambda} L(t)\rho_{\mathbf{n}-\mathbf{e}_\lambda}(t')L^\dagger(t') \\ & + \int_0^t dt' \sum_\lambda g_\lambda^2 e^{i\omega_\lambda(t-t')}(n_{1,\lambda}+1)L^\dagger(t')\rho_{\mathbf{n}+\mathbf{e}_\lambda}(t')L(t) \\ & + h.c. + O(g^4). \end{aligned} \tag{65}$$

Note that up to quadratic order in the coupling parameter we can replace $\rho_{\mathbf{n}}(t')$ by $\rho_{\mathbf{n}}(t)$ in Eq. (65) because the difference is of quadratic order.

Furthermore, provided that the spectrum of H_S is discrete, we can expand the coupling operators as

$$L(t) = \sum_\omega e^{-i\omega t}L(\omega) \tag{66}$$

$$L^\dagger(t) = \sum_\omega e^{i\omega t}L^\dagger(\omega) \tag{67}$$

where

$$L(\omega) = \sum_{\epsilon' - \epsilon = \omega} \Pi(\epsilon) L \Pi(\epsilon'). \tag{68}$$

Here $\Pi(\epsilon)$ denotes a projection operator onto the eigenspace of H_S corresponding to the eigenvalue ϵ. Substituting these expansions and transforming the integration variables from t' to $t - t'$, Eq. (65) can be written as

$$\begin{aligned}
\dot{\rho}_{\mathbf{n}}(t) = &- \sum_{\omega,\omega'} e^{i(\omega'-\omega)t} \sum_{\lambda} \Gamma_{d,\mathbf{n},\lambda}(t,\omega') L(\omega) L^{\dagger}(\omega') \rho_{\mathbf{n}}(t) \\
&- \sum_{\omega,\omega'} e^{i(\omega'-\omega)t} \sum_{\lambda} \Gamma_{u,\mathbf{n},\lambda}(t,\omega') \rho_{\mathbf{n}}(t) L^{\dagger}(\omega') L(\omega) \\
&+ \sum_{\omega,\omega'} e^{i(\omega'-\omega)t} \sum_{\lambda} \Gamma_{u,\mathbf{n}-\mathbf{e}_\lambda,\lambda}(t,\omega') L(\omega) \rho_{\mathbf{n}-\mathbf{e}_\lambda}(t) L^{\dagger}(\omega') \\
&+ \sum_{\omega,\omega'} e^{i(\omega'-\omega)t} \sum_{\lambda} \Gamma_{d,\mathbf{n}+\mathbf{e}_\lambda,\lambda}(t,\omega') L^{\dagger}(\omega') \rho_{\mathbf{n}+\mathbf{e}_\lambda}(t) L(\omega) \\
&+ h.c. + O(g^4)
\end{aligned} \tag{69}$$

for which we introduced the following notation

$$\Gamma_{u,\mathbf{n},\lambda}(t,\omega') = \int_0^t dt' e^{-i\omega' t'} g_\lambda^2 \left\langle b_\lambda(0) b_\lambda^{\dagger}(t') \right\rangle_{\mathbf{n}} \tag{70}$$

$$\Gamma_{d,\mathbf{n},\lambda}(t,\omega') = \int_0^t dt' e^{-i\omega' t'} g_\lambda^2 \left\langle b_\lambda^{\dagger}(t') b_\lambda(0) \right\rangle_{\mathbf{n}} \tag{71}$$

We recall from section 2.3 that if the typical time scale for the evolution of the system is large compared to $|\omega - \omega'|$, the oscillations average out over time allowing us to neglect them unless $\omega = \omega'$. Under this assumption Eq. (69) reduces to

$$\begin{aligned}
\dot{\rho}_{\mathbf{n}}(t) = &- i \sum_{\omega,\lambda} S_{d,\mathbf{n},\lambda}(t,\omega) \left[L(\omega) L^{\dagger}(\omega), \rho_{\mathbf{n}}(t) \right] \\
&- i \sum_{\omega,\lambda} S_{u,\mathbf{n},\lambda}(t,\omega) \left[L^{\dagger}(\omega) L(\omega), \rho_{\mathbf{n}}(t) \right] \\
&- \tfrac{1}{2} \sum_{\omega,\lambda} \gamma_{d,\mathbf{n},\lambda}(t,\omega) \left\{ L(\omega) L^{\dagger}(\omega), \rho_{\mathbf{n}}(t) \right\} \\
&- \tfrac{1}{2} \sum_{\omega,\lambda} \gamma_{u,\mathbf{n},\lambda}(t,\omega) \left\{ L^{\dagger}(\omega) L(\omega), \rho_{\mathbf{n}}(t) \right\} \\
&+ \sum_{\omega,\lambda} \gamma_{u,\mathbf{n}-\mathbf{e}_\lambda,\lambda}(t,\omega) L(\omega) \rho_{\mathbf{n}-\mathbf{e}_\lambda}(t) L^{\dagger}(\omega) \\
&+ \sum_{\omega,\lambda} \gamma_{d,\mathbf{n}+\mathbf{e}_\lambda,\lambda}(t,\omega) L^{\dagger}(\omega) \rho_{\mathbf{n}+\mathbf{e}_\lambda}(t) L(\omega) \\
&+ O(g^4)
\end{aligned} \tag{72}$$

where we defined

$$\gamma_{d,\mathbf{n},\lambda}(t,\omega) = \Gamma_{d,\mathbf{n},\lambda}(t,\omega) + \Gamma_{d,\mathbf{n},\lambda}^{*}(t,\omega) \tag{73}$$

$$\gamma_{u,\mathbf{n},\lambda}(t,\omega) = \Gamma_{u,\mathbf{n},\lambda}(t,\omega) + \Gamma_{u,\mathbf{n},\lambda}^{*}(t,\omega) \tag{74}$$

as well as

$$S_{d,\mathbf{n},\lambda}(t,\omega) = \frac{1}{2i}\left(\Gamma_{d,\mathbf{n},\lambda}(t,\omega) - \Gamma^*_{d,\mathbf{n},\lambda}(t,\omega)\right) \tag{75}$$

$$S_{u,\mathbf{n},\lambda}(t,\omega) = \frac{1}{2i}\left(\Gamma_{u,\mathbf{n},\lambda}(t,\omega) - \Gamma^*_{u,\mathbf{n},\lambda}(t,\omega)\right). \tag{76}$$

We will refer to the coupled set of differential equations described by Eq. (72) as the *hierarchy*. Note that although each layer of the hierarchy is similar to a master equation of Lindblad-type, it is not really in this form. The reason for this is that the right hand side of Eq. (72) depends not only on $\rho_{\mathbf{n}}$ but also on other matrices.

Although the hierarchy is attractive from a theoretical perspective because it does not involve the Born approximation or the assumption that the bath is Markovian, it also has its disadvantages. One problem is that when one is interested in using the master equation numerically, it is inevitable to take some cut-off in the hierarchy. How such a cut-off can be taken consistently will be discussed in section 4.1. However, still we are left with very many matrices that we are forced to take into account since the number of matrices required grows with the number of bath modes. This problem can be mitigated slightly by restricting our attention to fluctuations around an initial thermal state for the bath as we show in section 4.1 but still solving these equations is significantly more time-consuming than solving a single master equation.

3.3 GENERALISED LINDBLAD FORM

Comparing the discussion in section 2.6 to the derivation of the hierarchy in the previous sections, one might expect it to be possible to write our equations in generalised Lindblad form. If this were the case, it would have the advantage of guaranteeing that our equations give rise to trace-preserving and completely positive dynamics. Moreover, in this section we show that to bring Eq. (72) into generalised Lindblad form approximations would have to be done that cannot be justified.

The most general form for which we know the dynamics to be completely positive and trace-preserving is the scenario where the rates in the generalised Lindblad-form are time-dependent but positive. Indeed, supposing the rates to be positive, we would be able to write Eq. (72) in generalised Lindblad form as defined in Eq. (50) provided that we take the $H^{\mathbf{n}}$ to be

$$\begin{aligned} H^{\mathbf{n}} = &\sum_{\omega,\lambda} S_{d,\mathbf{n},\lambda}(t,\omega) L(\omega) L^\dagger(\omega) \\ &+ \sum_{\omega,\lambda} S_{u,\mathbf{n},\lambda}(t,\omega) L^\dagger(\omega) L(\omega), \end{aligned} \tag{77}$$

and the non-zero entries of R to be

$$R_{1,\omega}^{\mathbf{n},\mathbf{n}-\mathbf{e}_\lambda}(t) = \sqrt{\gamma_{d,\mathbf{n},\lambda}(t,\omega)}L(\omega), \tag{78}$$

$$R_{1,\omega}^{\mathbf{n},\mathbf{n}+\mathbf{e}_\lambda}(t) = \sqrt{\gamma_{u,\mathbf{n}+\mathbf{e}_\lambda,\lambda}(t,\omega)}L^\dagger(\omega). \tag{79}$$

To see why this works, it should be noted that

$$\gamma_{u,\mathbf{n}-\mathbf{e}_\lambda,\lambda}(t,\omega) = \gamma_{d,\mathbf{n},\lambda}(t,\omega). \tag{80}$$

However, the assumption that the decay rates are positive does not hold. After all, the decay rates are multiples of some time-dependent complex exponential integrated over time.

Furthermore, we cannot, as is usually done to obtain an equation in Lindblad form, take the upper bound of the time integrals to infinity at each level of the hiearchy yielding constant and positive rates. This is due to the fact that the rates are not superpositions of oscillating terms whose sum decays, but consist of a single oscillating term with nothing to interfere with. This can be seen from the formulas above by noting that the rates corresponding to the different oscillators are equal to two times the real part of

$$\int_0^t dt' e^{-i\omega' t'} g_\lambda^2 \left\langle b_\lambda(0) b_\lambda^\dagger(t') \right\rangle_{\mathbf{n}} \tag{81}$$

whereas there is only one rate if we assume the Born approximation that is given by

$$\int_0^t dt' e^{-i\omega' t'} \sum_\lambda g_\lambda^2 \left\langle b_\lambda(0) b_\lambda^\dagger(t') \right\rangle_{\mathbf{0}}. \tag{82}$$

The superposition in Eq. (81) is what allows the integrand to decay quickly with time due to interference effects between different frequencies. From the fact that we have a single oscillation in Eq. (82) it is clear that no such cancellation effects can occur, which prevents us from taking the long time limit. This leads us to the conclusion that the hierarchy derived in section 3.2 cannot be brought into generalised Lindblad form.

This does not mean however, that it is not possible at all to derive a master equation in generalised Lindblad form from first principles, it only means that the Fock basis for the environment is not the right tool to do so. In fact, master equations in Lindblad form have been derived [12, 15, 16]. There are two important differences between our approach and the one taken in [12] which we would like to clarify. Firstly, for the numerical implementation in [12] it is assumed that the coupling operators of the environment are Gaussian orthogonal random matrices whereas we couple the system to the bath with quantum mechanical raising and lowering operators. Secondly, the basis used to describe the environment in [12] is the energy eigenbasis. Why the basis is an important factor in the success can be seen as follows. If we consider the conditioned time evolution for the system where the bath is in a given energy eigenstate, it may be a superposition of many Fock states. These in turn can give rise to the superpositions in the integrands of the rates that are necessary to take the long time limit and arrive at a master equation in generalised Lindblad form. However, using the energy eigenbasis for the environment in the model we consider in this thesis is far from straightforward.

3.4 IMPOSING THE BORN APPROXIMATION

Verifying that the hierarchy reduces to the usual Lindblad-type master equation if we impose the Born-Markov approximation is an important consistency check of the hierarchy derived in section 3.2 which we perform in this section. The method by which we do so however, also hints towards a possible generalisation of the Born approximation as introduced in section 3.5.

To impose the Born approximation on the hierarchy we introduce the following ansatz:

$$\rho_{\mathbf{n}}(t) = \frac{e^{-\beta\sum_\mu \omega_\mu n_\mu}\rho_S(t)}{\sum_{\mathbf{m}} e^{-\beta\sum_\mu \omega_\mu m_\mu}}. \tag{83}$$

It supposes the environment to be in a thermal state at an inverse temperature β which does not change as the system evolves. Imposing this ansatz for the case where the environment starts in a thermal state with inverse temperature β is therefore equivalent to enforcing the Born approximation.

Now that the different levels of the hierarchy no longer depend on different matrices, the hierarchy can be summed over to obtain a master equation for $\rho_S(t)$. To be more precise, by plugging in the ansatz from Eq. (83) into Eq. (72) and summing over $\mathbf{n}$ we obtain a closed form equation for $\rho_S(t)$. The resulting equation includes terms of the form

$$\frac{\sum_{\mathbf{n}} n_\lambda e^{-\beta\sum_\mu \omega_\mu n_\mu}}{\sum_{\mathbf{m}} e^{-\beta\sum_\mu \omega_\mu m_\mu}}. \tag{84}$$

This expression represents the expectation value of the number operator of a single bath oscillator which is given by

$$\overline{n}_\lambda(\beta) := \frac{1}{e^{\beta\omega_\lambda} - 1} \tag{85}$$

as is reviewed in appendix A. The resulting equation for the reduced density matrix reads

$$
\begin{aligned}
&\dot{\rho}_S(t) = \sum_{\mathbf{n}} \dot{\rho}_{\mathbf{n}}(t) = \\
&- i \sum_{\omega} \int_0^t dt' \mathrm{Im}\left[\alpha^+(t', \omega, \beta)\right] \left[L(\omega)L^\dagger(\omega), \rho_S(t)\right] \\
&- i \sum_{\omega} \int_0^t dt' \mathrm{Im}\left[\alpha^-(t', \omega, \beta)\right] \left[L^\dagger(\omega)L(\omega), \rho_S(t)\right] \\
&- \sum_{\omega} \int_0^t dt' \mathrm{Re}\left[\alpha^+(t', \omega, \beta)\right] \left\{L(\omega)L^\dagger(\omega), \rho_S(t)\right\} \\
&- \sum_{\omega} \int_0^t dt' \mathrm{Re}\left[\alpha^-(t', \omega, \beta)\right] \left\{L^\dagger(\omega)L(\omega), \rho_S(t)\right\} \\
&+ 2 \sum_{\omega} \int_0^t dt' \mathrm{Re}\left[\alpha^-(t', \omega, \beta)\right] L(\omega)\rho_S(t)L^\dagger(\omega) \\
&+ 2 \sum_{\omega} \int_0^t dt' \mathrm{Re}\left[\alpha^+(t', \omega, \beta)\right] L^\dagger(\omega)\rho_S(t)L(\omega) \\
&+ O(g^4), \qquad (86)
\end{aligned}
$$

where we defined

$$\alpha^+(t', \omega, \beta) = \sum_{\lambda} g_\lambda^2 e^{-i(\omega-\omega_\lambda)t'} \overline{n}_\lambda(\beta), \qquad (87)$$

$$\alpha^-(t', \omega, \beta) = \sum_{\lambda} g_\lambda^2 e^{-i(\omega-\omega_\lambda)t'} (\overline{n}_\lambda(\beta) + 1), \qquad (88)$$

which represent the correlation functions of the bath.

Thus far we have imposed the Born approximation, but have made no assumption on the Markovianity of the bath yet. Recall that we called a bath Markovian if the correlation functions drop of quickly with respect to the time scales over which $\rho_S(t)$ changes, which is used to justify taking the limit of the upper bound of the integrals in Eq. (86) to ∞. Again we stress that this approximation on the integral is only truly valid if the spectrum of the system is continuous as otherwise we always have some finite recurrence time. Therefore we replace the finite model for the bath with one with a continuous spectrum, which guarantees irreversibility, such that the dynamics before the recurrence time of the finite model is identical.

The bath only influences the reduced system dynamics via its correlation functions in the perturbative equation that we derived, which makes it sufficient to find a continuum model that accurately reproduces these before the recurrence time. In practice, the replacement of a finite bath model can be achieved by replacing the sums over λ by an integral over ω and g_λ^2 by a function $J(\omega)$ called the spectral density. To see how this can be consistent, note that

$$J(\omega) = \sum_{\lambda} g_\lambda^2 \delta(\omega - \omega_\lambda) \qquad (89)$$

gives the same result as the finite bath. With this choice of $J(\omega)$ one could rightly argue that we have not changed anything. However, we can approximate $J(\omega)$ with an actual function as long as the correlation functions do not change significantly and we nevertheless end up with a continuous spectrum and irreversibility.

Supposing we can find some $J(\omega)$ that accurately describes the influence of the bath on the system dynamics, we can take the long time limit on the integrals, which, using

$$\int_0^\infty e^{\pm i\omega t'} dt' = \pm i\mathcal{P}\frac{1}{\omega} + \pi\delta(\omega), \tag{90}$$

gives

$$\begin{aligned}
\alpha^+(t,\omega,\beta) &= \pi J(\omega)\overline{n}(\beta,\omega) + i\mathcal{P}\int_0^\infty d\tilde{\omega}\frac{J(\tilde{\omega})}{\tilde{\omega}-\omega}\overline{n}(\beta,\tilde{\omega}) \\
\alpha^-(t,\omega,\beta) &= \pi J(\omega)(\overline{n}(\beta,\omega)+1) + i\mathcal{P}\int_0^\infty d\tilde{\omega}\frac{J(\tilde{\omega})}{\tilde{\omega}-\omega}(\overline{n}(\beta,\tilde{\omega})+1),
\end{aligned}$$

where

$$\overline{n}(\beta,\omega) = \frac{1}{e^{\beta\omega}-1}. \tag{91}$$

Using the relations above, Eq. (86) can be reduced to

$$\begin{aligned}
\dot{\rho}_S(t) = &- i[H_{LS},\rho_S(t)] \\
&- \pi\sum_\omega J(\omega)\overline{n}(\beta,\omega)\left\{L(\omega)L^\dagger(\omega),\rho_S(t)\right\} \\
&- \pi\sum_\omega J(\omega)(\overline{n}(\beta,\omega)+1)\left\{L^\dagger(\omega)L(\omega),\rho_S(t)\right\} \\
&+ 2\pi\sum_\omega J(\omega)(\overline{n}(\beta,\omega)+1)L(\omega)\rho_S(t)L^\dagger(\omega) \\
&+ 2\pi\sum_\omega J(\omega)\overline{n}(\beta,\omega)L^\dagger(\omega)\rho_S(t)L(\omega) \\
&+ O(g^4),
\end{aligned} \tag{92}$$

where

$$\begin{aligned}
H_{LS} = &\sum_\omega \mathcal{P}\int_0^\infty d\tilde{\omega}\frac{J(\tilde{\omega})}{\tilde{\omega}-\omega}\overline{n}(\beta,\tilde{\omega})L(\omega)L^\dagger(\omega) \\
&+ \sum_\omega \mathcal{P}\int_0^\infty d\tilde{\omega}\frac{J(\tilde{\omega})}{\tilde{\omega}-\omega}(\overline{n}(\beta,\tilde{\omega})+1)L^\dagger(\omega)L(\omega)
\end{aligned} \tag{93}$$

is usually referred to as the Lamb shift Hamiltonian.

This shows how the master equation in Lindblad form derived in section 2.3 can be derived from the hierarchy by invoking the Born approximation.

3.5 GENERALISING THE BORN APPROXIMATION

The master equation in Lindblad form from section 3.4 has certain advantages compared to the hierarchy we introduced in section 3.2. For example, we know from section 2.1 and section 2.2 that the master equation in Lindblad form preserves fundamental physical properties, whereas we have no such guarantee for the weak-coupling hierarchy. Furthermore, the master equation in Lindblad form is easier to solve numerically. The difference in numerical complexity is mainly due to the fact that the number of density matrices we need to compute for the hierarchy grows with the number of particles and the number of excitations allowed as we discuss in section 4.1. However, the master equation in Lindblad form also has disadvantages compared to our hierarchy. Since we used the Born approximation in its derivation, it does not allow the bath to change its state, an assumption that we expect to fail when we consider systems far from equilibrium. In this section we propose a compromise between the generality of the hierarchy and the desirable properties of the master equation in Lindblad form by introducing what we call the *generalised Born approximation*.

The generalised Born approximation assumes that the environment remains in a thermal state throughout the evolution, but is allowed to change its temperature, i.e.

$$\rho_{tot}(t) = \rho_S(t) \otimes \frac{e^{-\beta'(t) H_B}}{\mathrm{Tr}_B \left[e^{-\beta'(t) H_B} \right]}. \tag{94}$$

This condition can be imposed on the hierarchy by substituting

$$\rho_{\mathbf{n}}(t) = \frac{e^{-\beta'(t) \sum_\mu \omega_\mu n_\mu} \rho_S(t)}{\mathrm{Tr}_S \sum_{\mathbf{m}} e^{-\beta'(t) \sum_\mu \omega_\mu m_\mu} \rho_S(t)}. \tag{95}$$

Other than being a straightforward generalisation of the Born approximation, this ansatz can be motivated by considering the results presented in [2]. In this paper a system consisting of a single harmonic oscillator is considered that is coupled via a Caldeira-Legett spectral density to an environment consisting of harmonic oscillators. The paper shows analytically that in the weak coupling limit the system evolves to a thermal state, albeit at a temperature that is not necessarily equal to the initial temperature of the bath. This thermalisation to a temperature different from the initial one is incompatible with the Born approximation but not the generalisation proposed here.

Imposing the generalised Born approximation on the hierarchy by substituting the ansatz from Eq. (95), we can repeat the procedure of resumming the hierarchy to obtain an expression nearly identical to Eq. (86). The only difference between the equation we obtain and Eq. (86) is that the constant inverse bath temperature β is replaced by a time-dependent inverse bath temperature $\beta'(t)$. Thus by imposing the generalised Born approximation we have reduced the hierarchy to a time-local master equation in Lindblad form with a time-dependent generator. This time-local master equation can be more solved more efficiently numerically than the hierarchy because we now again only need one density matrix. Furthermore, the fact that we now have a time-local master equation with time-dependent Lindblad generator forms the starting point for showing desirable properties similar to those satisfied by equations in Lindblad form as discussed in section 3.6.

3.6 PROPERTIES OF THE GENERALISATION

Thus far we have derived a Lindblad-type master equation where the time-dependence of the elements from the decoherence matrix comes from the time-dependence of the bath temperature. The number of equations however, is still not big enough to determine the evolution of all the variables which necessitates the imposition of an additional constraint on the dynamics. In this section however, we do not discuss candidates for this constraint to which we devote section 3.8. Instead we suppose that a constraint has been found that fixes the dynamics and satisfies $\beta'(t) > 0$ at all times and discuss the general properties that the master equation with the time-dependent temperature satisfies under this assumption.

From the discussion in chapter 2 we can draw the following conclusions about the generalised master equation we derived:

- It preserves hermiticity and the trace because it is a Lindblad-type master equation.
- Under the assumption that $\beta'(t) > 0$ at all times, it preserves complete positivity becacuse the elements of the decoherence matrix are positive.
- It does not generate a quantum dynamical semi-group because the elements of the decoherence matrix are time-dependent.
- The change in entropy is non-negative at every point in time because it is a time-dependent Markovian master equation.

Thus the Lindblad-like master equation we derived satisfies the most important physical properties while being more general than a master equation in Lindblad form.

3.7 STEADY STATE IN THE LONG TIME LIMIT

Generally, open quantum systems in contact with a large environment approach a thermal state in the long time limit provided that the coupling is sufficiently weak. This is consistent with the predictions of the Born-Markov master equations provided that there are no conservation laws prohibiting thermalisation. In this section we assume that $\beta'(\infty)$ exists to show that in the long time limit a thermal state of the system is a steady state solution, provided that it has the same temperature as the environment. Although this is not equivalent to showing that a thermal state is approached, it is a necessary condition that has to be satisfied.

A general thermal state for the system at some a priori unspecified temperature β' is given by

$$\rho_S^{\mathrm{th}} = \frac{e^{-\beta' H_S}}{\mathrm{Tr}_S\left[e^{-\beta' H_S}\right]}. \tag{96}$$

Before plugging in this equation as an ansatz into the master equation derived using the generalised Born approximation, we note that

$$\rho_S^{th} L(\omega) = e^{\beta'\omega} L(\omega) \rho_S^{th} \tag{97}$$

$$\rho_S^{th} L^\dagger(\omega) = e^{-\beta'\omega} L^\dagger(\omega) \rho_S^{th} \tag{98}$$

as a result of the definition for $L(\omega)$. From these relations we see that

$$\left[\rho_S^{\mathrm{th}}, H_{LS}\right] = 0 \tag{99}$$

as well as

$$\left\{L(\omega)L^\dagger(\omega), \rho_S^{\mathrm{th}}\right\} = e^{\beta'\omega} L(\omega) \rho_S^{\mathrm{th}} L^\dagger(\omega) \tag{100}$$

$$\left\{L^\dagger(\omega)L(\omega), \rho_S^{\mathrm{th}}\right\} = e^{-\beta'\omega} L^\dagger(\omega) \rho_S^{\mathrm{th}} L(\omega). \tag{101}$$

From Eq. (100) and Eq. (101) we conclude that our thermal state ansatz is a solution provided that

$$\overline{n}(\beta_\infty, \omega) = (\overline{n}(\beta_\infty, \omega) + 1) e^{-\beta'\omega}. \tag{102}$$

This condition is satisfied if and only if $\beta' = \beta_\infty$, which shows that a thermal state of the system with the temperature of the bath is a solution in the long time limit.

3.8 IMPOSING ENERGY CONSERVATION

The generalised Born approximation introduces a new unknown, the inverse temperature of the bath, for which an additional requirement on the system has to be imposed in order to fix it. In this section we discuss if energy conservation of the total system can fulfil this role. After all, the violation of energy conservation due to the Born approximation, as discussed in section 2.5, was the main motivation for us to study generalisations of the Born approximation in the first place.

Energy conservation of the total system is usually imposed by required that

$$0 = \frac{d}{dt}\mathrm{Tr}\left[H\rho(t)\right] \tag{103}$$

where $\rho(t)$ is the density matrix of the total system. One could plug in the assumption from Eq. (94) which gives

$$0 = \frac{d}{dt}\mathrm{Tr}\left[H\left(\rho_S(t)\otimes\frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}_B\left[e^{-\beta'(t)H_B}\right]}\right)\right]. \tag{104}$$

Introducing the following notation for clarity

$$\langle ... \rangle_S := \mathrm{Tr}_S\left[...\rho_S(t)\right] \tag{105}$$

$$\langle ... \rangle_B := \mathrm{Tr}_B\left[...\frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}_B\left[e^{-\beta'(t)H_B}\right]}\right] \tag{106}$$

allows us to write Eq. (104) as

$$\begin{aligned} 0 = &\frac{d}{dt}\langle H_S\rangle_S \\ &- \dot{\beta}'(t)\left[\langle H_S\rangle_S\langle H_B\rangle_B + \langle H_B^2\rangle_B\right] \\ &+ \dot{\beta}'(t)\left[\langle H_S\rangle_S + \langle H_B\rangle_B\right]\langle H_B\rangle_B. \end{aligned} \tag{107}$$

Note that in the above we used $\mathrm{Tr}_S\left[\dot{\rho}_S(t)\right] = 0$, which holds because the evolution equation for the reduced density matrix is a Linblad-like master equation. Thus $\dot{\beta}'(t)$ can now be written as

$$\dot{\beta}'(t) = \frac{\frac{d}{dt}\langle H_S\rangle_S}{\langle H_B^2\rangle_B - \langle H_B\rangle_B^2}. \tag{108}$$

Here the denominator in Eq. (108) is the variance of the bath energy which can be explicitly calculated as shown in appendix A.

An important check for the consistency of our equations is that the generalisation of the Born approximation that we propose does not violate preservation of the trace of the total system. This can be seen explicitly by considering

$$1 = \mathrm{Tr}\left[\rho_S(t)\otimes\frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}_B\left[e^{-\beta'(t)H_B}\right]}\right]. \tag{109}$$

Taking the derivative with respect to time gives

$$0 = \frac{d}{dt}\langle I\rangle_S - \beta'(t)\langle I\rangle_S\langle H_B\rangle_B + \beta'(t)\langle I\rangle_S\langle H_B\rangle_B\langle I\rangle_B, \tag{110}$$

where I denotes the unit operator. Thus we see that Eq. (110) reduces to $0 = 0$ showing that the total trace is conserved.

An important step after deriving a master equation is determining its domain of validity. In order to see when the system of equations introduced in this section is expected to produce results different from the standard second order equation using the Born approximation, let us consider the bath temperature $\beta'(t)$, which by integrating Eq. (108), can be written as

$$\beta'(t) = \beta + \int_0^t dt' \frac{\frac{d}{dt}\langle H_S \rangle_S}{\langle H_B^2 \rangle_B - \langle H_B \rangle_B^2}. \tag{111}$$

From this we see that we expect different results if the change in energy of the system is comparable to the energy variance of the bath for non-negligible periods of time. If the bath is accurately described by the Born approximation, i.e. if its heat capacity is huge compared to the energy transfer, we should recover the results obtained using the Born-Markov master equation to high accuracy.

In summary, we have derived two equations, one time-local master equation in Lindblad-form with a time-dependent generator and a scalar equation determining the time evolution of the bath temperature. These equations are coupled since the master equation depends on $\beta'(t)$, and Eq. (108) depends on both the current temperature of the bath and the current reduced density matrix. Furthermore, we have imposed energy conservation on the total system and checked that the trace of the total system remains conserved. However, it turns out that although the condition for energy conservation that we get seems appealing[1], the resulting numerical predictions are not better than those predicted by the master equation in Lindblad form as we will see in chapter 4. To explain the failure of Eq. (111) as displayed in section 4.3, we now consider a subtle point in the derivation outlined above.

A more precise version of any ansatz that supposes the density matrix of the total system to be a product state should read like

$$\rho(t) = \rho_S(t) \otimes \rho_B(t) + h.o. \tag{112}$$

Here the higher order terms describe the entanglement that can be neglected in the weak coupling limit. We implicitly assumed that these higher order terms do not contribute. Although this is usually the case since we usually plug such an ansatz into a perturbative expansion whose leading order term is of second order. In this case however, if there terms linear in the coupling in Eq. (112), it could give rise to terms of second order in Eq. (104). Neglecting these terms introduces an inconsistency because we do keep the terms quadratic in the coupling arising from the derivative with respect to $\rho_S(t)$ in Eq. (107). This inconsistency is a possible explanation for the numerical results presented in section 4.3.

---

[1] Since the energy variance of a bosonic bath is equal to $k_B T^2$ times the heat capacity, Eq. (108) is consistent with the thermodynamic definition of the heat capacity.

To impose energy in a way more consistent with the perturbative approach we have chosen, we consider a second order perturbative expansion of $\frac{d}{dt}\langle H\rangle = 0$ before inserting our ansatz. To this end we note that we can consider the energy of the total system in the interaction picture, i.e.

$$\langle H\rangle = \mathrm{Tr}\left[H\rho(t)\right] = \mathrm{Tr}\left[H_I(t)\rho_I(t)\right]. \tag{113}$$

We emphasise that $\rho(t)$ denotes the density matrix of the total system and Tr denotes the trace over all degrees of freedom. Furthermore, we introduce the notation

$$H_I(t) = e^{iH_0t}He^{-iH_0t} \tag{114}$$

for the interaction picture Hamiltonian. Similarly,

$$\rho_I(t) = e^{-iH_0t}\rho(t)e^{iH_0t} \tag{115}$$

denotes the total density matrix in the interaction picture. Since we have been considering the density matrix to be in the interaction picture throughout this thesis, we drop the index I from now on.

Imposing energy conservation is then equivalent to requiring

$$0 = \frac{d}{dt}\langle H\rangle = \mathrm{Tr}\left[(H_0 + H_I(t))\frac{d}{dt}\rho(t)\right]. \tag{116}$$

To derive the final expression, we already used that we eventually plug in the generalised Born ansatz for the total density matrix, which is a product state between the reduced density matrix and a thermal state for the environment. This causes terms involving a product of an odd number of interaction picture Hamiltonians to vanish under the trace.

Since our goal is to find an equation that fixes $\beta'(t)$ from Eq. (116), we recall that in section 2.3 we derived the evolution of the total density matrix up to highest order in perturbation theory to be given by

$$\frac{d\rho(t)}{dt} = \frac{1}{i}\left[H_I(t), \rho(0)\right] - \int_0^t ds\left[H_I(t), \left[H_I(t-s), \rho(t-s)\right]\right]. \tag{117}$$

Plugging Eq. (117) into Eq. (116) gives

$$0 = -\int_{t_0}^t \mathrm{Tr}\left[H_0\left[H_I(t), \left[H_I(t-s), \rho(t-s)\right]\right]\right] \tag{118}$$

where we again used the fact that expectation values of odd factors of $H_I(t)$ do not concern us since we eventually plug in the generalised Born ansatz. Furthermore, we can replace $\rho(t-s)$ by $\rho(t)$ because the difference is of higher order.

Now that we have an equation expressing energy conservation at second order in perturbation theory we can plug in the generalised Born ansatz, which we recall to be given by

$$\rho(t) = \rho_S(t) \otimes \frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}\left[e^{-\beta'(t)H_B}\right]}. \tag{119}$$

Plugging this into Eq. (118) and simplifying the commutators using

$$L(t) = \sum_{\omega} e^{-i\omega t} L(\omega) \tag{120}$$

and employing the secular approxmation, we get

$$\begin{aligned}
0 =&\mathrm{Tr}\left[H_0\left(\sum_{\omega}\sum_{\lambda}\int_0^t ds g_{\lambda}^2 e^{i(\omega_\lambda-\omega)s}(L^\dagger(\omega)\rho_S(t)L(\omega)\otimes b_\lambda \frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}_B\left[e^{-\beta'(t)H_B}\right]} b_\lambda^\dagger)\right)\right]\\
&-\mathrm{Tr}\left[H_0\left(\sum_{\omega}\sum_{\lambda}\int_0^t ds g_{\lambda}^2 e^{i(\omega_\lambda-\omega)s}(L(\omega)L^\dagger(\omega)\rho_S(t)\otimes b_\lambda^\dagger b_\lambda \frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}_B\left[e^{-\beta'(t)H_B}\right]})\right)\right]\\
&+\mathrm{Tr}\left[H_0\left(\sum_{\omega}\sum_{\lambda}\int_0^t ds g_{\lambda}^2 e^{i(\omega_\lambda-\omega)s}(L(\omega)\rho_S(t)L^\dagger(\omega)\otimes b_\lambda^\dagger \frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}_B\left[e^{-\beta'(t)H_B}\right]} b_\lambda)\right)\right]\\
&-\mathrm{Tr}\left[H_0\left(\sum_{\omega}\sum_{\lambda}\int_0^t ds g_{\lambda}^2 e^{i(\omega_\lambda-\omega)s}(\rho_S(t)L^\dagger(\omega)L(\omega)\otimes \frac{e^{-\beta'(t)H_B}}{\mathrm{Tr}_B\left[e^{-\beta'(t)H_B}\right]} b_\lambda b_\lambda^\dagger)\right)\right]\\
&+h.c.
\end{aligned}$$

Thus far the calculation is the same as when one would try to derive a master equation. Now however, we also have the operator H_0 in the trace. Let us consider the two operators H_S and H_B that compose H_0 separately. If we consider the terms involving H_S, we note that taking the trace over the degrees of freedom of the environment is unaffected by its presence, so we simply get the trace over H_S times the time derivative of the reduced density matrix. For $H_B = \sum_\mu \omega_\mu b_\mu^\dagger b_\mu$ we consider the cases where μ is unequal or equal to λ separately. In the former case we get a scalar factor multiplied with the trace over the time derivative of the reduced density matrix which gives zero. In the latter case we get different combinations of creation and annihilation operators which gives rise to quadratic terms in the number operator, whose exact form we turn to now.

Taking the trace and replacing $\sum_{\omega_\lambda} g_\lambda^2$ by $\int d\tilde{\omega} J(\tilde{\omega})$ and taking the long time limit gives

$$
\begin{aligned}
0 &= \mathrm{Tr}_S\left[H_S \dot{\rho}_S(t)\right] \\
&+ \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{i(\tilde{\omega}-w)s} n(\beta',\tilde{\omega})(n(\beta',\tilde{\omega})-1)\tilde{\omega}\mathrm{Tr}\left[L^\dagger(\omega)\rho_S(t)L(\omega)\right] \\
&- \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{i(\tilde{\omega}-w)s} n(\beta',\tilde{\omega})^2\tilde{\omega}\mathrm{Tr}\left[L(\omega)L^\dagger(\omega)\rho_S(t)\right] \\
&+ \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{i(\tilde{\omega}-w)s} (n(\beta',\tilde{\omega})+1)^2\tilde{\omega}\mathrm{Tr}\left[L(\omega)\rho_S(t)L^\dagger(\omega)\right] \\
&- \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{i(\tilde{\omega}-w)s} (n(\beta',\tilde{\omega})+1)n(\beta',\tilde{\omega})\tilde{\omega}\mathrm{Tr}\left[\rho_S(t)L^\dagger(\omega)L(\omega)\right] \\
&+ \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{-i(\tilde{\omega}-w)s} n(\beta',\tilde{\omega})(n(\beta',\tilde{\omega})-1)\tilde{\omega}\mathrm{Tr}\left[L^\dagger(\omega)\rho_S(t)L(\omega)\right] \\
&- \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{-i(\tilde{\omega}-w)s} n(\beta',\tilde{\omega})^2\tilde{\omega}\mathrm{Tr}\left[L(\omega)L^\dagger(\omega)\rho_S(t)\right] \\
&+ \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{-i(\tilde{\omega}-w)s} (n(\beta',\tilde{\omega})+1)^2\tilde{\omega}\mathrm{Tr}\left[L(\omega)\rho_S(t)L^\dagger(\omega)\right] \\
&- \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{-i(\tilde{\omega}-w)s} (n(\beta',\tilde{\omega})+1)n(\beta',\tilde{\omega})\tilde{\omega}\mathrm{Tr}\left[\rho_S(t)L^\dagger(\omega)L(\omega)\right].
\end{aligned}
$$

This expression can be simplified by using the cyclicity of the trace which reduces it to

$$
\begin{aligned}
0 &= \mathrm{Tr}_S\left[H_S \dot{\rho}_S(t)\right] \\
&- \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{i(\tilde{\omega}-w)s} n(\beta',\tilde{\omega})\tilde{\omega}\mathrm{Tr}\left[L^\dagger(\omega)\rho_S(t)L(\omega)\right] \\
&+ \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{i(\tilde{\omega}-w)s} (n(\beta',\tilde{\omega})+1)\tilde{\omega}\mathrm{Tr}\left[L(\omega)\rho_S(t)L^\dagger(\omega)\right] \\
&- \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{-i(\tilde{\omega}-w)s} n(\beta',\tilde{\omega})\tilde{\omega}\mathrm{Tr}\left[L^\dagger(\omega)\rho_S(t)L(\omega)\right] \\
&+ \sum_\omega \int_0^\infty ds \int d\tilde{\omega} J(\tilde{\omega}) e^{-i(\tilde{\omega}-w)s} (n(\beta',\tilde{\omega})+1)\tilde{\omega}\mathrm{Tr}\left[L(\omega)\rho_S(t)L^\dagger(\omega)\right].
\end{aligned}
$$

Finally, we can make use of Eq. (90) to arrive at the following final expression.

$$
\begin{aligned}
0 &= \mathrm{Tr}_S\left[H_S \dot{\rho}_S(t)\right] \\
&- \sum_\omega 2\pi J(\omega) n(\beta',\tilde{\omega})\omega\mathrm{Tr}\left[L^\dagger(\omega)\rho_S(t)L(\omega)\right] \\
&+ \sum_\omega 2\pi J(\omega)(n(\beta',\omega)+1)\omega\mathrm{Tr}\left[L(\omega)\rho_S(t)L^\dagger(\omega)\right].
\end{aligned}
\tag{121}
$$

Here we can interpret the first term as the change of energy of the system and the remaining two terms as flow of energy to and from the bath respectively.

To simplify the second order energy conservation equation we recall that

$$L(\omega) = \sum_{\epsilon'-\epsilon=\omega} |\epsilon\rangle\langle\epsilon|L|\epsilon'\rangle\langle\epsilon| = \sum_{\epsilon'-\epsilon=\omega} L_{\epsilon\epsilon'}|\epsilon\rangle\langle\epsilon'| \tag{122}$$

$$L^{\dagger}(\omega) = \sum_{\epsilon'-\epsilon=\omega} |\epsilon\rangle\langle\epsilon|L^{\dagger}|\epsilon'\rangle\langle\epsilon| = \sum_{\epsilon'-\epsilon=\omega} L^{*}_{\epsilon'\epsilon}|\epsilon\rangle\langle\epsilon'| \tag{123}$$

where $|\epsilon\rangle$ refers to the energy basis of the system and we have introduced the following convention

$$L_{\epsilon\epsilon'} = \langle\epsilon|L|\epsilon'\rangle = \langle\epsilon'|L^{\dagger}|\epsilon\rangle^{*} = (L^{\dagger}_{\epsilon'\epsilon})^{*}. \tag{124}$$

Using these expansions it can be shown that the right hand side of Eq. (121) is actually zero regardless of β', i.e. energy is conserved up to second order regardless of the inverse temperature of the bath if we assume the initial state to be a product state. The generalised Born ansatz with time-dependent temperature is therefore consistent with energy conservation although imposing energy conservation does not fix the temperature of the bath.

3.9 DISCUSSION

In this chapter we have considered possible generalisations of the master equation in Lindblad form derived in chapter 2 for the model Hamiltonian introduced in Eq. (8). We showed that if the Born approximation is not invoked, the reduced density matrix is determined by an infinite system of coupled differential equations instead of a single master equation. Furthermore, we introduced an ansatz called the generalised Born approximation that allows the temperature of the environment to change over time. This ansatz allowed us to reduce the hierarchy to a Lindblad-type master equation. We showed that this master equation preserves the most important physical properties provided that the additional constraint required to fix the evolution of the bath temperature satisfies certain conditions. Finally, we considered two ways of imposing energy conservation of the total system which we aimed to use as a constraint to fix the newly introduced time-dependent bath temperature. The first way of imposing energy conservation results in a system of equations whose predictions reduce to those of the master equation in Linblad form in the limit where the bath is continuous, but they do not necessarily yield more accurate predictions away from this limit as we will show in chapter 4. We explained the failure of this constraint to produce better numerical predictions by arguing that its derivation is not consistent with our perturbative approach. The second way in which we imposed energy condition, which was fully consistent with our second order approach, showed that the generalised Born approximation is consistent with energy conservation provided that we assume the secular and the Markov approximation, but did not fix the temperature of the environment.

4

NUMERICAL TESTS

In this chapter we study the equations derived in chapter 3 from a numerical perspective. In section 4.1 we start with some general considerations regarding the system of equations determining the reduced density matrix, without relying on the Born approximation, derived in section 3.2. In particular, we consider the number of matrices required to solve the equations numerically for given cut-off parameters. In section 4.2 we discuss numerical results that indicate that in the limit where the number of modes in the environment diverges, the predictions obtained by numerically solving the hierarchy coincide with those obtained when solving the standard second order equation, whose derivation involves the Born approximation. By comparing to numerically exact results, we also evaluate its predictions in the case where the consists of few oscillators.

In section 4.3, we support the claim we made in section 3.8 that Eq. (108) is not the correct formula to determine the evolution of the inverse temperature of the bath. In the previous chapter we gave a general argument concerning the inconsistent use of perturbation theory, here we support it with numerical evidence instead.

4.1 TRUNCATING THE HIERARCHY

One may rightly wonder how the hierarchy involving infinitely many equations and infinitely many non-normalised density matrices can be solved numerically. The honest answer is that it cannot be done without further approximations. What can be done however, is solving a closely related problem where we introduced some cut-off, which, if chosen correctly, should make the solution of this new problem equivalent to solving the hierarchy up to the desired accuracy. In this section we discuss how this truncation can be performed and how it affects the number of non-normalised density matrices required to solve the problem numerically.

One way the hierarchy can be truncated is by imposing the restriction that each oscillator in the environment can have at most a fixed finite number of quanta d. A problem with this approach is that the number of non-normalised density matrices involved in the hierarchy then grows exponentially with the number of oscillators in the environment M, i.e. the number of non-normalised density matrices required to solve the truncated hierarchy numerically would be d^M. Furthermore, it is likely that there will be non-normalised density matrices that remain zero throughout the evolution which therefore do not play a role. Therefore we first discuss an alternative approach to deriving a hierarchy which we use to come to a smarter truncation scheme.

Recall that the model under consideration is that of a system coupled to a single thermal bath[1] initially. It turns out that this system can be equivalently modelled by the same quantum systems coupled to two identical baths at zero temperature using what is called a thermofield transform, see [17] and references therein. To be more precise, it transforms the model Hamiltonian we introduced in section 1.1 to

$$\begin{aligned} H = H_S + \sum_\lambda \omega_\lambda b_{1\lambda}^\dagger b_{1\lambda} + \sum_\lambda h_{1\lambda}(b_{1\lambda} L^\dagger + b_{1\lambda}^\dagger L) \\ - \sum_\lambda \omega_\lambda b_{2\lambda}^\dagger b_{2\lambda} + \sum_\lambda h_{2\lambda}(b_{2\lambda}^\dagger L^\dagger + b_{2\lambda} L) \end{aligned} \tag{125}$$

where $b_{1\lambda}$ and $b_{2\lambda}$ are the annihilation operators of the first and second bath respectively. The constants describing the coupling to both baths are given by

$$h_{1\lambda} = g_\lambda \sqrt{1 + \bar{n}_\lambda} \tag{126}$$

$$h_{2\lambda} = g_\lambda \sqrt{\bar{n}_\lambda} \tag{127}$$

In this new formulation of the problem, excitations in the first bath and second bath correspond to 'particles' and 'holes' in the environment we considered before doing the thermofield transform respectively. Let us discuss an example to clarify what we mean by this terminology. Consider a state for the environment where a given oscillator in the first bath has x excitations corresponds to a state for the environment in the picture before the thermofield transform where the same oscillator has x excitations on top of its thermal energy distribution.

In this case the reduced density matrix of the system can be composed similarly to before as

$$\rho_S(t) = \sum_{\mathbf{n}} \rho_{\mathbf{n}}(t) \tag{128}$$

where the only difference lies in the fact that now we have that $\mathbf{n} \in \mathbb{N}^{2M}$. In fact, the derivation from section 3.1 and 3.2 can be straightforwardly generalised to this case. If we introduce the following definitions

$$\gamma_{i,u/d,\mathbf{n}}(t,\omega) = \Gamma_{i,u/d,\mathbf{n}}(t,\omega) + \Gamma^*_{i,u/d,\mathbf{n}}(t,\omega) \tag{129}$$

$$S_{i,u/d,\mathbf{n}}(t,\omega) = \frac{1}{2i}\left(\Gamma_{i,u/d,\mathbf{n}}(t,\omega) - \Gamma^*_{i,u/d,\mathbf{n}}(t,\omega)\right) \tag{130}$$

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[1] Thus far we referred to the surroundings of the quantum system as its environment because it was only necessary to assume that it was in a thermal state initially at some points during the derivation. Here it essential throughout because it is a requirement to do the thermofield transform. Therefore we will use the term *bath* or *thermal bath* in this section.

where

$$\begin{aligned}
\Gamma_{1,u,\mathbf{n}}(t,\omega') &= \int_0^t dt' e^{-i\omega' t'} \sum_\lambda h_{1\lambda}^2 \left\langle b_{1\lambda}(0) b_{1\lambda}^\dagger(t') \right\rangle_{\mathbf{n}} \\
\Gamma_{1,d,\mathbf{n}}(t,\omega') &= \int_0^t dt' e^{-i\omega' t'} \sum_\lambda h_{1\lambda}^2 \left\langle b_{1\lambda}^\dagger(t') b_{1\lambda}(0) \right\rangle_{\mathbf{n}} \\
\Gamma_{2,u,\mathbf{n}}(t,\omega') &= \int_0^t dt' e^{i\omega' t'} \sum_\lambda h_{2\lambda}^2 \left\langle b_{2\lambda}(0) b_{2\lambda}^\dagger(t') \right\rangle_{\mathbf{n}} \\
\Gamma_{2,d,\mathbf{n}}(t,\omega') &= \int_0^t dt' e^{i\omega' t'} \sum_\lambda h_{2\lambda}^2 \left\langle b_{2\lambda}^\dagger(t') b_{2\lambda}(0) \right\rangle_{\mathbf{n}}
\end{aligned}$$

the resulting hierarchy we get from repeating the derivation consists of layers given by

$$\begin{aligned}
\dot{\rho}_{\mathbf{n}}(t) = &\sum_\omega \gamma_{1,u,\mathbf{n}-\mathbf{e}_{1\lambda}}(t,\omega) L(\omega) \rho_{\mathbf{n}-\mathbf{e}_{1\lambda}}(t) L^\dagger(\omega) \\
&+ \sum_\omega \gamma_{1,d,\mathbf{n}+\mathbf{e}_{1\lambda}}(t,\omega) L^\dagger(\omega) \rho_{\mathbf{n}+\mathbf{e}_{1\lambda}}(t) L(\omega) \\
&- i \sum_\omega S_{1,d,\mathbf{n}}(t,\omega) \left[L(\omega) L^\dagger(\omega), \rho_{\mathbf{n}}(t) \right] \\
&- i \sum_\omega S_{1,u,\mathbf{n}}(t,\omega) \left[L^\dagger(\omega) L(\omega), \rho_{\mathbf{n}}(t) \right] \\
&- \tfrac{1}{2} \sum_\omega \gamma_{1,d,\mathbf{n}}(t,\omega) \left\{ L(\omega) L^\dagger(\omega), \rho_{\mathbf{n}}(t) \right\} \\
&- \tfrac{1}{2} \sum_\omega \gamma_{1,u,\mathbf{n}}(t,\omega) \left\{ L^\dagger(\omega) L(\omega), \rho_{\mathbf{n}}(t) \right\} \\
&+ \sum_\omega \gamma_{2,d,\mathbf{n}+\mathbf{e}_{2\lambda}}(t,\omega) L(\omega) \rho_{\mathbf{n}+\mathbf{e}_{2\lambda}}(t) L^\dagger(\omega) \\
&+ \sum_\omega \gamma_{2.u,\mathbf{n}-\mathbf{e}_{2\lambda}}(t,\omega) L^\dagger(\omega) \rho_{\mathbf{n}-\mathbf{e}_{2\lambda}}(t) L(\omega) \\
&- i \sum_\omega S_{2,u,\mathbf{n}}(t,\omega) \left[L(\omega) L^\dagger(\omega), \rho_{\mathbf{n}}(t) \right] \\
&- i \sum_\omega S_{2,d,\mathbf{n}}(t,\omega) \left[L^\dagger(\omega) L(\omega), \rho_{\mathbf{n}}(t) \right] \\
&- \tfrac{1}{2} \sum_\omega \gamma_{2,u,\mathbf{n}}(t,\omega) \left\{ L(\omega) L^\dagger(\omega), \rho_{\mathbf{n}}(t) \right\} \\
&- \tfrac{1}{2} \sum_\omega \gamma_{2,d,\mathbf{n}}(t,\omega) \left\{ L^\dagger(\omega) L(\omega) \rho_{\mathbf{n}}(t) \right\} \\
&+ O(g^4). \qquad (131)
\end{aligned}$$

This thermofield-based hierarchy is the starting from which we discuss how a truncation procedure can be devised.

Recall that in section 3.3 we noticed that the hierarchy and master equations in generalised Lindblad form both amount to considering an extended state space when compared to master equations invoking the Born approximation. The generalised space considered for the hierarchy are the states in the combined Hilbert space of the system and environment where the bath itself is not entangled, i.e. its density matrix is diagonal. In particular, we stress that entanglement between the system and environment is allowed for. The idea of the cut-off method we introduce in the following is that we restrict the state space a bit more by only allowing for a certain number of fluctuations in the bath compared to its initial state.

Before discussing the general truncation procedure, we show how the equations that one usually derives using the Born approximation can be obtained from our this thermofield-based hierarchy, which is a specific case of the truncation procedure we discuss next. As a first step we recall that the Born approximation comes down to continually projecting the total system onto the subspace in Hilbert space for which the bath is in its thermal state. In this case we get

$$\mathcal{P}_0 \rho_S(t) = \mathcal{P}_0 \sum_{\mathbf{n}} \rho_{\mathbf{n}}(t) = \rho_{\mathbf{0}}(t) \tag{132}$$

where $\mathcal{P}_0$ denotes the projection operator onto the subspace of Hilbert space where the bath is in its vacuum state (the vacuum state corresponds to the initial thermal state of the physical system because of the thermofield transformation we did). Furthermore, we obtain a master equation for $\mathcal{P}_0 \rho_S(t)$ by applying the projection operator to the equation for the time derivative of $\rho_S(t)$

$$\dot{\rho}_{\mathbf{0}}(t) = \mathcal{P}_0 \dot{\rho}_S(t) = \mathcal{P}_0 \sum_{\mathbf{n}} \dot{\rho}_{\mathbf{n}}(t) \tag{133}$$

Noting that there are terms involving $\rho_{\mathbf{0}}(t)$ in both the time derivative of $\rho_{\mathbf{0}}(t)$ and the time derivative of the $\rho_{\mathbf{e}_{i,\lambda}}(t)$ we find that

$$\begin{aligned}
\dot{\rho}_{\mathbf{0}}(t) = & \sum_{\omega,\lambda} \gamma_{1,u,\mathbf{0},\lambda}(t,\omega) L(\omega) \rho_{\mathbf{0}}(t) L^\dagger(\omega) \\
& - i \sum_{\omega,\lambda} S_{1,u,\mathbf{0},\lambda}(t,\omega) \left[L^\dagger(\omega) L(\omega), \rho_{\mathbf{0}}(t) \right] \\
& - \tfrac{1}{2} \sum_{\omega,\lambda} \gamma_{1,u,\mathbf{0},\lambda}(t,\omega) \left\{ L^\dagger(\omega) L(\omega), \rho_{\mathbf{0}}(t) \right\} \\
& + \sum_{\omega,\lambda} \gamma_{2.u,\mathbf{0},\lambda}(t,\omega) L^\dagger(\omega) \rho_{\mathbf{0}}(t) L(\omega) \\
& - i \sum_{\omega,\lambda} S_{2,u,\mathbf{0},\lambda}(t,\omega) \left[L(\omega) L^\dagger(\omega), \rho_{\mathbf{0}}(t) \right] \\
& - \tfrac{1}{2} \sum_{\omega,\lambda} \gamma_{2,u,\mathbf{0},\lambda}(t,\omega) \left\{ L(\omega) L^\dagger(\omega), \rho_{\mathbf{0}}(t) \right\} \\
& + O(g^4)
\end{aligned} \tag{134}$$

which can be checked to agree with the weak-coupling master equation derived under the Born approximation before taking the long time limit, i.e. Eq. (26).

More generally, we can consider a continual projection onto the subspace of Hilbert space where the baths have at most n excitations denoted by $\mathcal{P}_n$. In this case, we take the density matrix under consideration to be given by

$$\mathcal{P}_n \rho_S(t) = \mathcal{P}_n \sum_{\mathbf{n}} \rho_{\mathbf{n}}(t) \tag{135}$$

where $\mathcal{P}_n$ reduces the range of the index set in the sum to the finite set of all vectors the sum of whose entries is smaller than or equal to n. To take only these environmental states into account consistently, the equation for $\dot{\rho}_{\mathbf{n}}(t)$ has to be adjusted if the sum of the entries of $\mathbf{n}$ is equal to n.

Let us consider a vector $\tilde{\mathbf{n}}$ with positive integer-valued entries whose sum is equal to n. In this case the expression for $\dot{\rho}_{\tilde{\mathbf{n}}}$ involves terms like $\rho_{\tilde{\mathbf{n}}+\mathbf{e}_{1\lambda}}$ and $\rho_{\tilde{\mathbf{n}}+\mathbf{e}_{2\lambda}}$, which, due to the assumption on $\tilde{\mathbf{n}}$, refer to states of the environment with $n+1$ excitations in the two baths combined. Therefore such terms are projected to zero under $\mathcal{P}_n$. However, there are also terms in the expression for $\mathcal{P}_n \dot{\rho}_S(t)$ that involve $\rho_{\tilde{\mathbf{n}}}$ which arise from $\dot{\rho}_{\mathbf{n}+\mathbf{e}_{1\lambda}}$ for example. We take these terms into account by adding them to the layer corresponding to $\tilde{\mathbf{n}}$ in analogy to what we got in Eq. (134). With these modifications, the hierarchy is reduced to a finite system of coupled differential equations which can be solved numerically.

However, as noted in section 3.2 the number of density matrices can become a problem as we consider many oscillators in the environment and/or a high cut-off. Let us first suppose that the initial temperature of the physical bath is unequal to zero. If we then allow for at most one excitation in the environment, the number of oscillators required[2] is $2M+1$. This is because we consider an additional density matrix corresponding for every possible excitation in the environment, for which there are $2M$ options. If we consider the case where we allow for two fluctuations, the situations already becomes a bit more difficult. In addition to the number of density matrices we had before we have $2M$ density matrices corresponding to the possibilities for a single oscillator in the environment to have two excitations and we get $M(2M-1)$ density matrices representing an environment that has two excitations shared by two different oscillators. If the initial bath is at zero temperature we can repeat the same arguments illustrated above only we have to replace $2M$ by M.

Using such combinatorial arguments, similar calculations can be done for the cases where we allow for even more excitations, but it should already be clear that the coupled system of differential equations grows very complex very quickly in this way. Still, we can choose to allow for few excitations which allows us to simulate large baths in contrast to the naive truncation procedure outlined at the start of this section which was plagued by an exponentially growing number of density matrices.

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[2] As before, M denotes the number of oscillators in the physical environment.

4.2 SOLVING THE HIERARCHY

In this section we discuss the numerical results obtained when solving the truncated hierarchy for two examples. The examples we consider are the Jaynes-Cummings and the damped Jaynes-Cummings model, which we introduced in section 1.3. We compare the numerical results obtained from the truncated hierarchy to those obtained from the exact solution and the second order equations which rely on the Born approximation, which corresponds to truncating the hierarchy to allow for no excitations in the environment as discussed in section 4.1.

Master equations whose derivation involves invoking the the Born approximation implicitly allow for fluctuations in the environment because in such cases the Born approximation is only invoked after a second order expansion. Nevertheless, a consequence of the Born approximation is that at each point in time the bath part of the total system state is projected back onto its initial state. The situations that we consider in this section, with environments consisting of few oscillators, were chosen to test the hierarchy because they represent situations where we expect effects due to the exchange of quanta between the system and the environment to be most pronounced.

4.2.1 *Solving the Jaynes-Cummings model*

To put the hierarchy, i.e. the system of system of equations defined by Eq. (72), to the test, we begin by considering an example for which we know the exact evolution equations so that we have a reliable result to compare the predictions of the truncated hierarchy to. The situation we consider is that of a two-level system coupled to a harmonic oscillator that is in its vacuum state initially, i.e. the Jaynes-Cummings model at zero temperature as described in section 1.3. We obtain the numerically exact solution in this case by numerically solving the scalar hierarchy, which is possible in this case is because it is naturally truncated due to the fact that there is at most one excitation in the total system and the number of excitations is conserved by the interaction. For the same reason, truncating the hierarchy at one possible excitation for the environment is not a restriction up to the order in perturbation theory that we consider.

We suppose that initially the two-level system is in an entangled state given by

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \tag{136}$$

i.e. the initial reduced density matrix of the two-level system is a matrix with all its entries equal to one half. In the case, where in addition we suppose that the frequency of the harmonic oscillator to which we couple the two-level system is equal to that of the latter, we get the results depicted in figure 1 and figure 2.

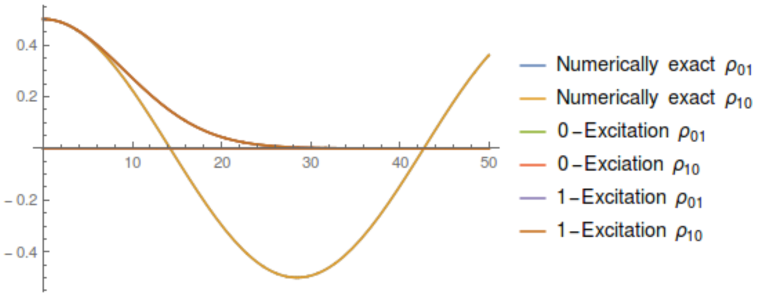

Figure 1: The off-diagonal elements of the reduced density matrix in the case where the environment consists of a single oscillator. The frequencies used to produce this plot are $\omega_0 = 3$ and $\omega = 3$, which represent the frequency of the two-level system and the environmental oscillator respectively. The coupling between the two-level system and its environmental oscillator is $g = 0.1$. The lines corresponding to the the 0-excitation and the 1-excitation case coincide.

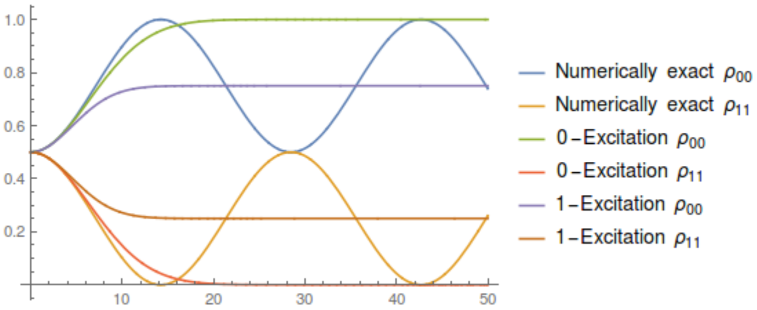

Figure 2: The diagonal elements of the reduced density matrix in the case where the environment consists of a single oscillator with parameters as described in figure 1. The prediction of the hierarchy in this case coincides with the mean value of the oscillations predicted by the exact solution.

The predictions of the truncated hierarchy allowing for one and zero excitations coincide for the non-diagonal entries. More interestingly, we see from figure 2 that if we do not allow the bath to fluctuate, we lose the quantum entirely, i.e. the total energy is not conserved. However, in the case where we allow for one excitation the quantum of energy that we start with does not disappear. Instead, it is eventually shared equally by the two-level system and the harmonic oscillator comprising the bath. The exact solution on the other hand does not predict quasi-equilibration, but predicts a continual oscillation that is captured by neither truncated version of the hierarchy.

4.2.2 *Increasing the number of cavity modes*

Let us now consider what happens if we add more resonant oscillators to the environment whilst keeping all the other parameters and the initial state the same. In figure 3 the results for the diagonal entries of the same problem that we considered before only now with five oscillators in the environment is shown. The predictions of the off-diagonal entries are again the same as those for the master equation that does not allow the environment to change.

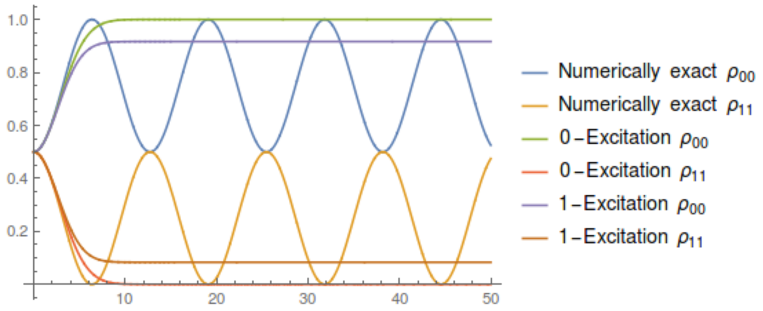

Figure 3: The off-diagonal elements of the reduced density matrix in the case where the environment consists of five identical oscillators. The frequencies used to produce this plot are $\omega_0 = 3$ and $\omega = 3$, which represent the frequencies of the two-level system and the environmental oscillators respectively. The coupling between the two-level system and the environmental oscillators is $g = 0.1$.

From figure 3 we see that the steady state approached by the truncated hierarchy allowing for one excitation changes with respect to the case where the environment consisted of a single oscillator. Instead of sharing its initial energy with one oscillator, it is distributed among all five oscillators in the environment and the two-level system itself. Thus we see that as we increase the number of oscillators in the environment, the predictions by the truncated hierarchy allowing for one excitation coincide increasingly with the predictions of the hierarchy where no excitations in the environment are allowed. This is consistent with the fact that for a larger environment the validity of the Born approximation increases. However, it can also be seen from figure 3 that the hierarchy allowing for one excitation now no longer predicts the correct mean value because the only change in the exact solution is that its oscillations have become more rapid.

The example considered thus far shows how due to allowing the environment to have excitations, the number of oscillators in the environment becomes an important variable. It also shows that there may still be important effects of the open system dynamics that are not captured by the hierarchy even with when the system is weakly coupled to the environment. More surprisingly, it turns out that there are cases where the predictions of the master equation that does not allow for fluctuations of the environment are better than a less truncated version of the hierarchy as show in the next section.

4.2.3 *Solving the damped Jaynes-Cummings model*

In this section we consider the damped Jaynes-Cummings model, which consists of a two-level system coupled to a continuous environment of harmonic oscillators as discussed in section 1.3. The spectral density, which is the continuous generalisation of the squares of the coupling parameters, is in this case given by

$$J(\omega) = \frac{1}{2\pi} \frac{\eta W}{(\omega - \omega_0)^2 + W^2}, \tag{137}$$

where η denotes the coupling strength, W determines the width of the Lorentzian, and ω_0 is the frequency of the two-level system. However, the number of degrees of freedom of the hierarchy and the scalar hierarchy diverge when considering a continuous environment so they cannot be solved in this case. Therefore we make use of a discretisation scehme that allows us to model the continuous environment with finitely many oscillators.

The idea behind discretisation schemes is that the spectral density determines the influence of the environment on the quantum system [18]. At least in the weak coupling case we see this in the fact that the influence of the environment on the system enters into the effective equations via

$$\int_0^t ds \sum_\lambda g_\lambda^2 e^{\pm i(\omega - \omega_\lambda)s}. \tag{138}$$

We aim to choose the frequencies and the couplings in such a way that it approximates

$$\int_0^t ds \int d\tilde{\omega} J(\tilde{\omega}) e^{\pm i(\omega - \tilde{\omega})s} \tag{139}$$

well before the revival time that depends on the number of oscillators chosen to model the continuous environment.

The easiest discretisation scheme imaginable is the one where we take an evenly spaced, i.e. linear, sampling of frequencies from the environment. Then we choose the coupling parameter g_λ corresponding to an oscillator of frequency ω_λ to be given by

$$\sqrt{J(\omega_\lambda)\Delta\omega} \tag{140}$$

where $\Delta\omega$ denotes the spacing between the discretised frequencies. Then

$$\sum_\lambda g_\lambda^2 = \sum_\lambda J(\omega_\lambda)\Delta\omega \approx \int d\tilde{\omega} J(\tilde{\omega} \tag{141}$$

because it is the Riemann sum corresponding to the integral.

For the simulations whose results are displayed in figure 4, we consider an environment consisting of twenty-one oscillators with evenly spaced frequencies between 2.5 and 3.5 such that $\Delta\omega = 0.05$. We take a linear sampling of the Lorentzian spectral density in Eq. (137) as described above. The remaining parameters we take to be $\eta = 0.1$, $W = 0.25$, and $\omega_0 = 3$ and the initial state we consider is one where the two-level system is in its excited state initially. Therefore the off-diagonal elements of the reduced density matrix are not of interest in this case.

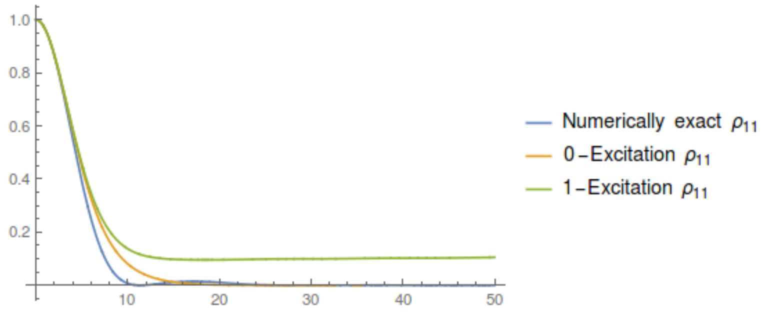

Figure 4: The probability of finding the two-level system in its excited state upon measurement.

As can be seen from figure 4, the truncation of the hierarchy allowing for quanta in the environmental oscillators predicts a steady state that is quantitatively different from the one predicted by the exact equations. The maximally truncated hierarchy, i.e. the hierarchy that does not allow for any excitations in the environment which is equivalent to the invoking the Born approximation, on the other hand does predict a steady state that is essentially the same as that predicted by the exact solution. By increasing the number of oscillators in the environment the predictions of the steady state in all three cases can be brought closer together, as discussed before, but this example clearly shows that considering a version of the hierarchy that allows for more entanglement between the system and environment does not necessarily give rise to more accurate results.

Based on the numerical results we conclude that the Born approximation is consistent with the perturbative expansion up to second order. Going beyond the Born approximation without increasing the order of the perturbative expansion does not produce more accurate results.

4.3 TESTING THE GENERALISED BORN APPROXIMATION

In the previous section, we saw that the numerical predictions of the (truncated) hierarchy allowing for excitations in the bath are not an improvement when compared to the predictions made by the standard second order master equation. Thus far we have however not yet numerically tested the system of equations resulting from the hierarchy by using the generalised Born approximation and the initial method of imposing energy conservation as discussed in section 3.8. Therefore we devote this section to the numerical predictions of this approach when considering quantum Brownian motion.

To be able to use the system of equations derived using the generalised Born approximation, it is necessary to assume that the initial temperature is non-zero. Otherwise the variance of the bath energy is zero making the time derivative of the inverse temperature of the bath diverge. This assumption is not very restrictive as no environment can ever truly reach its vacuum state. Therefore the situation in which we are troubled by this divergence is never really relevant. As a result of this non-zero temperature, it is no longer efficient to use the scalar hierarchy to obtain the numerically exact solution. Instead we use make use of the exact diagonalisation procedure outlined in Appendix B for the rest of this section.

Using the exact diagonalisation procedure necessitates the introduction of a cut-off for the oscillators, i.e. a maximal number of excitations each oscillator is allowed to have. For the results presented in this section we take this cut-off to be twenty-five. As in the previous section we take the coupling to the environment to be described by a Lorentzian spectral density which we again sample linearly using the same sampling range and number of oscillators. Also we take W, η, and ω_0 as before. The only other difference other than considering a harmonic oscillator as the system instead of a two-level system is that we now consider an initial state where the system has ten excitations and we consider the environment to be in a thermal state at a temperature equal to 0.5. The predictions for the expectation value of the number operator for the three different approaches under consideration here, and for the parameters specified above, are displayed in figure 5.

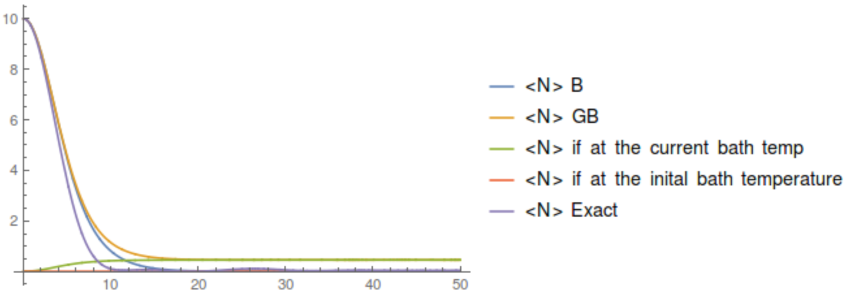

Figure 5: The expectation value of the number operator for the harmonic oscillator comprising the system at a given time as predicted by the three different approaches considered.

Note that figure 5 displays not only the time evolution of the expectation value for the number operator, but also the value of the number operator if the harmonic oscillator comprising the system were in a thermal state at temperature β or $\beta'(t)$. The system of equations associated to the generalised Born approximation, denoted by GB in the legend, predicts that the expectation value of the number operator approaches the thermal expectation value at temperature $\beta'(t)$. The same holds for the master equation associated to the Born approximation, denoted by B in the legend, provided that we replace $\beta'(t)$ by β in the above. The difference between these two cases however, is that $\beta'(t)$ decreases due to the transfer of energy from the system to the environment which raises the temperature of the latter, which is in line with our predictions from section 3.8. Nevertheless, the prediction from the exact diagonalisation procedure clearly again shows that the equations associated to the Born approximation are more accurate.

In the light of our general considerations regarding the inconsistency in the use of perturbation theory in section 3.8, it should not surprise us that the system of equations corresponding to the generalised Born approximation does not produce more accurate results than the standard second order equations. Nevertheless, the possibility that the numerical failure illustrated in this section is in fact (partially) due to the same issue that caused the numerical predictions of the truncated hierarchy to fail to produce more accurate results cannot be excluded.

5

CONCLUSION

In this thesis we have studied energy conservation in quantum systems with a discrete spectrum coupled linearly to an environment of harmonic oscillators. In order to do so, we have explored the possibility of describing open quantum systems without the Born approximation or by using a generalisation of the Born approximation.

We showed that a semi-infinite coupled system of differential equations, dubbed the hierarchy, can be derived that determines the reduced density matrix up to second order using a perturbative expansion but without relying on the Born approximation. The most important difference between the hierarchy and the usual second order time-local master equations is that it allows for an arbitrary amount of entanglement between the system and the environment at least up to second order. In order to solve the hierarchy numerically, we showed how the hierarchy can be truncated consistently. Surprisingly, the numerical tests we did show that the predictions of the (truncated) hierarchy are not necessarily more accurate than those of the usual second order master equation. This means not only that the Born approximation is fully consistent with the second order perturbative expansion but also that going beyond the Born approximation without considering higher order terms in the perturbative expansion does not give rise to more accurate predictions. This synergy between the Born approximation and the second order approach has, to the best of our knowledge, not been described in the literature.

Starting from the hierarchy we derived another generalisation of the usual second order master equation by introducing a generalised Born approximation, which allowed us to resum the hierarchy to a time-local master equation. Like the Born approximation, it supposes that the density matrix of the total system in second order terms can be written as a product state where the environment is in a thermal state, but now this temperature is allowed to be time-dependent. The introduction of this additional degree of freedom necessitates the imposition of an additional constraint in order to keep the problem from being undetermined. We showed that, after taking the long time limit and the secular approximation, the resulting master equation satisfies most of the properties that master equation in Lindblad form do, e.g. it preserves the trace and hermiticity of the reduced density matrix as well as complete positivity, provided that the constraint determining the evolution of the temperature of the environment does not allow this temperature to become non-positive. We considered energy conservation of the total system as the additional constraint required to make the system of equations fully determined.

Our initial approach prescribes the rate of change of the inverse temperature of the bath to be given by the transfer of energy at this moment divided by the variance of the energy of the bath at this time. This result is consistent with what would have been obtained if regular thermodynamics were used to describe the change of temperature of the environment. Although in the limit where the environment consists of infinitely many oscillators we argued it to give rise to the same results as those predicted by the Born approximation, we saw that away from this limit its predictions were not necessarily more accurate. We explained this failure to produce more accurate predictions by pointing to a subtlety in the derivation that shows that this initial approach is not consistent with the perturbative approach if the perturbative expression for total density matrix contains terms linear in the coupling.

In order to avoid this problem we considered a perturbative expansion for the total energy which allowed us to impose the generalised Born approximation consistently. It turns out that in this case the total energy is conserved up to second order for our generalised master equation, regardless of the temperature of the environment, provided that we use the secular and Markov approximations in the second order expansion for the derivative of the total system energy. This means that this approximative way of imposing energy conservation, i.e. including the secular and Markov approximations, does not function as a constraint that determines the evolution of the temperature of the environment. Also, this shows that the master equation in Lindblad form corresponding to the model we consider is consistent with energy conservation, provided that we use the aforementioned approximations. If we do not invoke these approximations energy conservation is not necessarily satisfied. This means that the weak coupling master equation does not conserve energy and that its departure from energy conservation becomes more relevant the less accurate the secular and Markovian approximations are.

Our findings lead naturally to a number of interesting questions and possible generalisations which we discuss in chapter 6.

6

OUTLOOK

In the master project presented here we have initiated a detailed study of energy conservation and its role in the theory of open quantum systems. From the results we have obtained, a number of directions for further research present themselves. Some of them are:

- We found that if we do not invoke the Markov and secular approximations energy conservation is in general not satisfied by second order master equations. It would therefore be interesting to investigate if this failure to satisfy energy conservation could be used to quantify the validity of the Markov and the secular approximation.
- Can energy conservation play a role if the system is truly irreversible, i.e. if the system is continuous, or can it only ever be relevant for finite environments?
- Do the conclusions we arrived at for the harmonic environment considered in this thesis change if we were to consider an environment consisting of anharmonic oscillators instead of harmonic ones?
- We have shown that the second order hierarchy allowing for more fluctuations in the environment does not outperform the second order master equation due to the synergy between the Born approximation and the second order approach. What has not been explored however, is if this conclusion is still valid if we include higher order perturbative terms into account in the hierarchy. To this end we note that the procedure by which we obtained the hierarchy, outlined in section 3.2, gives a straightforward recipe for obtaining the higher order generalisations.

A

PROPERTIES OF BOSONIC BATHS

The effect of the bath on an open quantum system is usually encoded in the effective equations for the system by expectation values of certain bath operators and the spectral density. Such expectation values can most easily be calculated by using the partition function as a generating functional. In this section we review this method and demonstrate how the bath observables used throughout the thesis can be determined.

We consider the case where the environment consists of harmonic oscillators with a discrete set of frequencies, i.e. the case where the Hamiltonian is given by

$$H_B = \sum_\lambda \omega_\lambda b_\lambda^\dagger b_\lambda = \sum_\lambda \omega_\lambda n_\lambda. \tag{142}$$

As before, b_λ and $b_\lambda^\dagger$ represent annihilation and creation operators satisfying the canonical commutation relations.

If we assume the bath to be in a thermal state at inverse temperature β, the partition function for a given oscillator is given by

$$Z_\lambda = \sum_{n_\lambda} e^{-\beta\omega_\lambda n_\lambda} = \frac{1}{1 - e^{-\beta\omega_\lambda}}. \tag{143}$$

Since the oscillators are independent, the partition function of the total system is given by

$$Z = \prod_\lambda Z_\lambda. \tag{144}$$

The partition function of the total system acts as a generating functional from which we can derive all the relevant expectation values, as we will show next.

As an example, let us consider the expectation value of the number operator of a given oscillator, which is given by

$$\langle n_\lambda \rangle = \frac{1}{Z} \prod_\mu \sum_{n_\mu} n_\lambda e^{-\beta \sum_\mu \omega_\mu n_\mu}. \tag{145}$$

From the expression above we can note that it can also be expressed as

$$\langle n_\lambda \rangle = -\frac{1}{\beta} \frac{\partial}{\partial \omega_\lambda} \ln Z. \tag{146}$$

Knowing this, $\langle n_\lambda \rangle$ can be easily computed using Eq. (143) and Eq. (144), which gives

$$\langle n_\lambda \rangle = \frac{e^{-\beta\omega_\lambda}}{1 - e^{-\beta\omega_\lambda}} = \frac{1}{e^{\beta\omega_\lambda} - 1}. \tag{147}$$

Similarly, we see that the expectation value of the energy of a given oscillator is given by

$$\langle H_\lambda \rangle = -\frac{\partial}{\partial \beta} \ln Z_\lambda = \frac{\omega_\lambda}{e^{\beta \omega_\lambda} - 1}, \tag{148}$$

from which it follows that the total energy of the bath is equal to

$$\langle H_B \rangle = \sum_\lambda \langle H_\lambda \rangle = \sum_\lambda \frac{\omega_\lambda}{e^{\beta \omega_\lambda} - 1}. \tag{149}$$

The final expectation value we are interested in is the variance of the energy, which is given by

$$\Delta H_B = \langle H_B^2 \rangle - \langle H_B \rangle^2 \tag{150}$$

Noting that

$$\begin{aligned} -\frac{\partial}{\partial \beta} \langle H_B \rangle &= \frac{\partial^2}{\partial \beta^2} \ln Z = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} - \left(\frac{1}{Z} \frac{\partial Z}{\partial \beta} \right)^2 \\ &= \langle H_B^2 \rangle - \langle H_B \rangle^2 \end{aligned} \tag{151}$$

allows us to compute the variance of the energy from Eq. (149) which gives

$$\Delta H_B = \sum_\lambda \frac{\omega_\lambda^2 e^{\beta \omega_\lambda}}{(e^{\beta \omega_\lambda} - 1)^2}. \tag{152}$$

This concludes our discussion of the case where describe the environment with a discrete set of oscillators.

To describe our finite system as a continuous system, we start from the Hamiltonian, which we rewrite as

$$H = \sum_k \omega_k b_k^\dagger b_k = \int d\tilde{k} g(\tilde{k}) \omega_{\tilde{k}} b_{\tilde{k}}^\dagger b_{\tilde{k}} \tag{153}$$

with

$$g(\tilde{k}) = \sum_k \delta(\tilde{k} - k) \tag{154}$$

Noting the similarity of the procedure above with how the spectral density was introduced, we might suppose that g can be approximated by an actual function instead of a distribution as long as the integrals we are interested in coincide in both cases.

Doing a transformation from wave vectors to frequencies, we can obtain a expression which allows us to replace sums over k by integrals over the frequency. First changing the delta functions to frequencies gives

$$g(\tilde{k}) = \sum_k \delta(\omega_{\tilde{k}} - \omega_k) \left| \frac{\partial \tilde{k}}{\partial \omega} \right|^{-1} \tag{155}$$

Then taking into account the transformation of the integral over k to an integral over ω gives

$$g(\omega) = \sum_k \delta(\omega_{\tilde{k}} - \omega_k). \tag{156}$$

In summary, if we want to replace a sum over wave vectors by some integral, we replace

$$\sum_k \to \int d\tilde{k} g(\tilde{k}), \tag{157}$$

$$\sum_k \to \int d\omega g(\omega), \tag{158}$$

with $g(\tilde{k})$ and $g(\omega)$ as above.

Using this we partition function can be written as

$$\ln Z = \int d\omega g(\omega) \ln \left[\frac{1}{e^{\beta\omega} - 1} \right] \tag{159}$$

The result we would then get for the variance is

$$\Delta E_B = \int_0^\infty d\omega g(\omega) \frac{\omega^2 e^{\beta\omega}}{(e^{\beta\omega} - 1)^2} \tag{160}$$

B

EXACT DIAGONALISATION

For a certain class of Hamiltonians quadratic in creation and annihilation operators analytic expressions for expectation values of operators in terms of the initial conditions can be found. The main idea of this method is to find a basis of creation and annihilation operators in terms of which the Hamiltonian is diagonal using what is called a Bogoliubov transformation. In the diagonal basis the time-dependence is well-known. To then make predictions about expectation values of operators, we expand them in the diagonal basis, plug in the time-dependence, and transform back to our original basis. Taking the expectation value afterwards leaves us with the desired expression in terms of the initial conditions. In this section we state only the results that are relevant to the discussion in section 3.8 and not give an overview of the general theory of diagonalisation, for which we refer the reader to [19] on which we based this appendix.

The general form of a Hamiltonian quadratic in the creation and annihilation operators is

$$H = \sum_{i,j=1}^{n} (\alpha_{ij} c_i^\dagger c_j + \tfrac{1}{2}\gamma_{ij} c_i^\dagger c_j^\dagger + \tfrac{1}{2}\gamma_{ji}^* c_i c_j). \tag{161}$$

The Hamiltonian we considered throughout this thesis is of this form provided that we take $\gamma_{ij} = 0$ for all i and j as well as

$$\alpha_{ij} = \begin{cases} g_{j-i} & \text{if } i \leq n_s \text{ and } j > n_S \\ g_{i-j} & \text{if } j \leq n_s \text{ and } i > n_S \\ 0 & \text{otherwise} \end{cases} \tag{162}$$

where n denotes the number of harmonic oscillators in the total system and n_S denotes the number of oscillators in the system part.

The Hamiltonian can be formulated differently if we define a vector of operators given by

$$\psi^T = \begin{pmatrix} c_1 & \dots & c_n & c_1^\dagger & \dots & c_n^\dagger \end{pmatrix} \tag{163}$$

as well as a $2n \times 2n$ matrix given by

$$M = \begin{pmatrix} \alpha & 0 \\ 0 & \alpha^T \end{pmatrix}. \tag{164}$$

Here the zeros in the definition of M denote $n \times n$ matrices. As a result, we can write the Hamiltonian as

$$H = \frac{1}{2}\psi^\dagger M \psi. \tag{165}$$

To eventually find a basis in terms of creation and annihilation operators such that the Hamiltonian is diagonal, we introduce a general transformation

$$c = Ad + Bd^{\dagger} \tag{166}$$

where d and $d^{\dagger}$ are again assumed to be creation and annihilation operators, i.e. they satisfy the canonical commutation relations. In terms of the matrix formulation that we introduced before, this corresponds to

$$\psi = T\varphi \tag{167}$$

where φ is defined analogously to ψ, only with the c's replaced with d's and T is given by

$$T = \begin{pmatrix} A & B \\ B^{*} & A^{*} \end{pmatrix}. \tag{168}$$

To ensure that T does indeed map onto bosonic creation and annihilation operators the requirement that T is unitary has to be imposed.

The problem of diagonalisation is now to find a matrix T that satisfies the conditions above which at the same time makes $T^{\dagger}MT$ diagonal so that

$$H = \frac{1}{2}\varphi^{\dagger}T^{\dagger}MT\varphi \tag{169}$$

is diagonal. It turns out that $\gamma_{ij} = 0$ for all i and j is a sufficient condition for the existence of such a matrix and it can be constructed explicitly [19]. Therefore we will assume from now on that T is known to us.

To obtain an expression for the expectation for the number operator of one of the system oscillators we start by expanding the creation and annihilation operators in terms of the diagonal basis, which gives

$$\begin{aligned} c_i(t) &= \sum_{k=1}^{n} a_{ik}d_k(t) + \sum_{k=1}^{n} b_{ik}d_k^{\dagger}(t) \\ &= \sum_{k=1}^{n} a_{ik}d_k(0)e^{-i\omega_k t} + \sum_{k=1}^{n} b_{ik}d_k^{\dagger}(0)e^{i\omega_k t}. \end{aligned} \tag{170}$$

Here a_{ik} and b_{ik} are the entries of the matrices A and B. Whenever we want to compute an expectation value of a combination of creation and annihilation operators, we substitute the expansion from Eq. (170) and its hermitian conjugate after which we substitute expressions for $d_k(0)$ and $d_k^{\dagger}(0)$ in terms of the original creation and annihilation operators. The equation for the $d_k(0)$ in terms of the original operators is given by

$$d_k(0) = \sum_{k=1}^{n} a_{ki}^{*}c_k(0) + \sum_{k=1}^{n} b_{ki}c_k^{\dagger}(0) \tag{171}$$

The result of the procedure outlined above is

$$\begin{aligned}c_i(t) = &\sum_{k=1}^{n} a_{ik}e^{-i\omega_k t}\left(\sum_{l=1}^{n} a_{lk}^{*}c_l(0) + \sum_{l=1}^{n} b_{lk}c_l^{\dagger}(0)\right)\\ &+ \sum_{k=1}^{n} b_{ik}e^{i\omega_k t}\left(\sum_{l=1}^{n} a_{kl}c_l^{\dagger}(0) + \sum_{l=1}^{n} b_{kl}^{*}c_l(0)\right). \end{aligned} \tag{172}$$

It turns out that in the specific case we consider, Eq. (172) can be simplified. To this end we consider the Heisenberg equation of motion for $c_k(t)$ which reads

$$\begin{aligned}\frac{dc_k(t)}{dt} &= i[H, c_k(t)]\\ &= i\sum_{r,s=1}^{n} \alpha_{rs}[c_r^{\dagger}c_s, c_k]\\ &= i\sum_{r,s=1}^{n} \alpha_{rs}\left(c_r^{\dagger}[c_s, c_k] + [c_r^{\dagger}, c_k]c_s\right)\\ &= i\sum_{s=1}^{n} \alpha_{ks}c_s(t). \end{aligned} \tag{173}$$

From Eq. (172) we see that we can also write $c_i(t)$ as

$$c_k(t) = \sum_{l=1}^{n} f_{kl}(t)c_l(0) + \sum_{l=1}^{n} g_{kl}(t)c_l^{\dagger}(0) \tag{174}$$

Combining this with Eq. (173) we see that

$$\frac{dg_{kl}(t)}{dt} = 0, \tag{175}$$

which, combined with the initial condition that $g_{kl}(0) = 0$, implies that $g_{kl}(t) = 0$. This reduces Eq. (172) to

$$\begin{aligned}c_i(t) = &\sum_{k,l=1}^{n} a_{ik}e^{-i\omega_k t}a_{lk}^{*}c_l(0)\\ &+ \sum_{k,l=1}^{n} b_{ik}e^{i\omega_k t}b_{kl}^{*}c_l(0)\end{aligned} \tag{176}$$

Now that we have expressions for the creation and annihilation operators in terms of the initial conditions, we turn to the quantity that we use to test the equations derived using the generalised Born approximation which is the expectation value of the number operator. In order to efficiently express $\langle c_i^{\dagger}(t)c_i(t)\rangle$ in terms of the initial conditions, we introduce matrices $A(t), \tilde{A}, B(t)$ and $\tilde{B}$ whose entries are given by

$$A_{ij}(t) = a_{ij}e^{-i\omega_j t} \tag{177}$$

$$\tilde{A}_{ij}(t) = a_{ij} \tag{178}$$

$$B_{ij}(t) = b_{ij}e^{i\omega_j t} \tag{179}$$

$$\tilde{B}_{ij}(t) = b_{ij} \tag{180}$$

This allows us to re-express Eq. (176) as

$$\begin{aligned} c_i(t) = &\sum_{l=1}^{n}\left(\tilde{A}(t)A^\dagger\right)_{il} c_l(0) \\ &+\sum_{l=1}^{n}\left(\tilde{B}(t)B^\dagger\right)_{il} c_l(0) \end{aligned} \tag{181}$$

Using this, we find

$$\begin{aligned} \langle c_i^\dagger(t)c_i(t)\rangle = &\sum_{l,s=1}^{n}\left(\tilde{A}(t)A^\dagger\right)_{il}\left(\tilde{A}(t)A^\dagger\right)^*_{is}\langle c_s^\dagger(0)c_l(0)\rangle \\ &+\sum_{l,s=1}^{n}\left(\tilde{A}(t)A^\dagger\right)_{il}\left(\tilde{B}(t)B^\dagger\right)^*_{is}\langle c_s^\dagger(0)c_l(0)\rangle \\ &+\sum_{l,s=1}^{n}\left(\tilde{B}(t)B^\dagger\right)_{il}\left(\tilde{A}(t)A^\dagger\right)^*_{is}\langle c_s^\dagger(0)c_l(0)\rangle \\ &+\sum_{l,s=1}^{n}\left(\tilde{B}(t)B^\dagger\right)_{il}\left(\tilde{B}(t)B^\dagger\right)^*_{is}\langle c_s^\dagger(0)c_l(0)\rangle. \end{aligned}$$

Since we assume in our model that the bath is in a thermal state initially, we have that

$$\langle c_s^\dagger(0)c_l(0)\rangle = \delta_{r,s}\langle N_r(0)\rangle \tag{182}$$

provided that $r, s \geq n_S$. If we assume that the initial state of the system is a statistical mixture as well, we get

$$\begin{aligned} \langle c_i^\dagger(t)c_i(t)\rangle = &\sum_{l=1}^{n}\left|\tilde{A}(t)A^\dagger\right|^2_{il}\langle c_l^\dagger(0)c_l(0)\rangle \\ &+\sum_{l=1}^{n}\left(\tilde{A}(t)A^\dagger\right)_{il}\left(\tilde{B}(t)B^\dagger\right)^*_{il}\langle c_l^\dagger(0)c_l(0)\rangle \\ &+\sum_{l=1}^{n}\left(\tilde{B}(t)B^\dagger\right)_{il}\left(\tilde{A}(t)A^\dagger\right)^*_{il}\langle c_l^\dagger(0)c_l(0)\rangle \\ &+\sum_{l=1}^{n}\left|\tilde{B}(t)B^\dagger\right|^2_{il}\langle c_l^\dagger(0)c_l(0)\rangle. \end{aligned} \tag{183}$$

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