Time development in open quantum systems

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Abstract

The purpose of this thesis is to examine the temporal evolution of open quantum systems, and to give the reader an introduction to this field. We will discuss why this can not be treated in the same manor as the evolution of closed systems, and I will provide an overview of some of the alternatives. In particular it will be emphasized that some of these have a non-Markovian character while others are Markovian. We will discuss the conditions under which these descriptions may be applied, and they will be illustrated using two very simple models of open systems: an open two-level system and an open harmonic oscillator. These models will also be used to illustrate particular characteristics that open systems have relative to closed ones, such as decay, damping, heating and decoherence.

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Contents

Chapter 1

Introduction

Since the 1920s the successes of Quantum mechanics have been many and substantial. It has allowed for the successful description, understanding and prediction of a vast list of phenomenons originating in the microscopic world. This list includes among several others such things as chemical reactions and molecular structure, the interactions between light and matter as applied for instance in a laser, as well as the electronic properties of different materials. That is, for instance the characteristics of conductors, semiconductors and insulators.

It has also allowed us to understand different forms of radioactive decay and other nuclear processes, the behavior and organization of the smallest building blocks of our universe: the elementary particles, and the crucially important processes occurring in the universe in the earliest moments after its creation. It is clear that when it comes to describing the world of the very small, Quantum mechanics gives the rules by which one must play. In later years, there has also been increasing experimental evidence of manifestly quantum mechanical concepts, such as superposition and entanglement, applying also to macroscopic objects at sufficiently low temperatures.

Quantum mechanics is an abstract formalism that provides a set of rules by which it is possible to determine the observable values of different properties of physical systems, as well as the probabilities for observing each of these values. Given appropriate knowledge of the internal interactions of the system, it can also predict the temporal development of these probabilities. In almost all cases quantum mechanics can only predict probabilities of observations, and it is thus a manifestly indeterministic theory. Quantum mechanics also strongly suggests that no useful improvement of this indeterminism is possible. Also, as long as it remains correct in its predictions and one has sufficient knowledge of the relevant interactions, quantum mechanics can in principle answer any question about nature that is experimentally testable.

The rules of quantum mechanics is thus seen to be a tool of overwhelming power in the investigations of a physicist interested in the microscopic world, and also obviously to a chemist or material scientist. However, in several cases it is important to take into account a crucial point concerning these rules: The fundamental postulates of quantum mechanics (as they are known) are formulated under the assumption that the physical system to be described is closed. That is, it it is assumed that the physical system does not interact at all with the rest of the world. In particular this applies, as we will see, to the postulate of time development.

In the very limited sense that standard quantum mechanics does allow for an external environment (that is, an additional system not included in the model), it is assumed that this environment can be described using classical physics. In this case, although the environment may have a strong effect on the quantum system to be analyzed, it is not itself affected in return. An example of the later case would be an atom placed in a laser beam, where the beam can be described as a classical electromagnetic field, which is not at all affected by the behavior of the quantum mechanical atom.

It is not hard to see that this is never a truly realistic assumption. Except for maybe the entirety of the universe, any physical system has an environment, and it is *always* interacting with it. Being both affected by it and affecting it back in return. Rather than this assumption ever being truly fulfilled, its justification is instead that the interaction with the environment can often be assumed to be so weak

that the quantum object will not be significantly affected during the timescales over which important properties are determined. In some cases however, even this will not be the case and it becomes necessary to in some way take the effects of the environment more explicitly into account. Such cases are referred to as open, and it is these and the theory and methods used for describing them that this text will be devoted to.

When the interactions between a quantum object and its environment becomes significant, they may have many important and interesting consequences. The environment may absorb energy from the object, a phenomenon which is seen for instance when an atom emits a photon of light, or in the even more familiar case of friction. Obviously, this flow of energy could also go the other way. In addition, random influences from the environment could cause the quantum object to undergo diffusion and thus dramatically change its characteristic motion over long timescales.

Another consequence of openness, which unlike the previous ones is exclusive to quantum mechanics is that of decoherence. In the most general meaning of the word decoherence is the transition from pure states to mixed states due to entanglement with the environment. It has been noted by Zurek[15] that this often picks out a particular set of states that are 'more classical' than others. Thus, decoherence could in many ways be said to be the process by which a quantum object 'looses its quantumness'. An understanding of this process is therefore very important for instance in relation to technological applications that rely heavily on the properties of quantum mechanics.

In this thesis I will examine in particular the time development of open systems. The major difference between the temporal evolutions of open and closed systems is precisely that open systems undergo decoherence: pure states do not nescessarily remain pure. This means that the theory of open systems can not be formulated in the standard formalism of state vectors, but must instead be described in terms of the more general state operator formalism. More importantly it means that the time development of open systems is not unitary, and thus these systems do not obey the time development postulate of standard quantum mechanics. It thus becomes a natural question what we are to replace this with in the theory of open systems. This is in a way the main question to be treated by the thesis.

We will encounter several alternative generalizations of this postulate. Some of these will generalize the postulate only in its integral form (which simply states that a quantum mechanical state develops unitarily) and some will generalize the corresponding differential form, that is the Schrödinger equation (or the Liouville equation in the state operator formalism). A major point will be that these can be classified as either Markovian or non-Markovian descriptions of the time development: A Markovian description is a description where it is explicitly assumed that the future states can be determined from the present one. A non-Markovian description is a description where this is not necessarily the case, so that information about the entire past may be needed.

The development of a closed quantum system is Markovian, but it is not hard to see that open quantum systems very well might need a non-Markovian description. This is because the environment will be able to store information about the objects past. If this information is only available in the environment, and later leaks back into the system then clearly the resulting state of the system can not be determined in a Markovian fashion. From these arguments alone we would expect that time development in open systems must almost exclusively be described in a non-Markovian manor. But the situation is not as bad as this: We will see that open systems can often be described Markovianly in a way that is even 'exact', in the sense that it is in agreement with a unitary model of a total system consisting of the open system plus an environment.

This exact Markovian description does however not always exist, and it must in any case be derived from a non-Markovian description which is again 'exact'. The general non-Markovian descriptions can be seen to apply to all models, but we must typically make some assumptions about the initial state. The non-Markovian framework is thus seen to indeed be the most general, whereas the Markovian one is simpler to apply and has a more intuitive interpretation. The later is particular the case in connection with a particular Markovian approximation scheme known as the *Lindblad equation*.

In addition to the Markovian and non-Markovian character of the time development, I will also briefly discuss some further characteristics of this development relative to closed systems. As mentioned this

includes things like decay and incoherent transfer, frictional damping and other forms of energy loss, heating and cooling as well as decoherence and Zureks 'Pointer basis' concept. Particularly the later is something I would have liked to give much more attention. In particular I would have liked to include a chapter on the role that this plays in connection with the quantum classical border, which has long been a particular interest of mine. Sadly however, I have not been able to devote any space for this very interesting subject, as I have instead chosen to focus mainly on the fundamental description of the time development, and in particular on the issue of Markovian versus non-Markovian descriptions.

Having introduced the subjects that will be discussed in the thesis, I will now provide a short outline of its organization. The main text is divided into two parts: Part I, which deals with general descriptions of time development in open systems, and Part II in which I threat two concrete models for purposes of illustration. In addition to this, chapter 2 contains some necessary prerequisite material which is typically not included in first courses on quantum mechanics. The most important elements are the density operator formalism, some mathematical formalism required for the description of composite systems, and finally some notes about the coherent state representation of harmonic oscillators.

Part I consists of three chapters. In chapter 3.1 I introduce the questions connected to the time development of open systems, and I discuss the first attempt to generalize the time development postulate of closed systems: namely the Kraus decomposition. In chapter 4 I discuss the Markovian frameworks for describing open systems, while in chapter 5 I discuss a particular non-Markovian framework. Part of this chapter will actually be devoted to discussing how this description can be used to derive an exact Markovian description that applies in many cases.

Part II contains only two chapters, each of which contains a treatment of one particular model. In chapter 6 I will discuss a simple model of an open two-level system. This model is something that is included in many standard texts on quantum mechanics in order to discuss in the simplest possible model the phenomenon of decay. The typical assumption about such decay is that it is exponential, and this is something that I will look into. The model of chapter 6 is also the one that will mainly be used to illustrate the different Markovian and non-Markovian descriptions of time development.

The model of chapter 7, which is a very simple model of a harmonic oscillator, will mainly be used to illustrate additional characteristics of open systems: We will here see an example of mechanical damping, effects of finite temperature, and also we will study decoherence. In particular we will look at two examples of Zurek's so called 'pointer bases'. A major part of the chapter will be devoted to the calculation of an exact solution, so that we can see how this is distinguished in particular from a particular Markovian approximation scheme.

Finally, in chapter 8 I will give a review of the conclusions and discussions that arose during the main text. I will also discuss some arising questions, and further work that could have been done if more time had been available.

Chapter 2

Prerequisite material

The reader of this thesis is assumed to have a basic understanding of quantum mechanics to the degree one would have after at least one introductory course on the subject. It is assumed that he/she is familiar with the fundamental postulates of the theory in their standard formulation, Hilbert spaces and the mathematics of these, and also with Dirac's Bra-ket notation. In this thesis we will however encounter certain concepts that go beyond the standard subjects of introductory courses. This includes in particular the coherent state representation of harmonic oscillators, the formalism of density operators as well as concepts such as tensor product and partial trace, which are connected to the description of composite systems. In order for the reader to have a basic understanding also of these subjects before he/she begins reading the main text, I will provide a short explanation of the necessary prerequisites in this chapter.

2.1 Density operator formalism

As the reader should be familiar with, the standard description of quantum mechanical states are in terms of wave functions or state vectors. However, the accessible knowledge about a quantum system can not always be parametrized by such a state, which is frequently referred to as a 'pure' state. Consider for instance a situation where a system is prepared either in a state $|a\rangle$ or $|b\rangle$ with 50% probability for each, and where the actual result is unknown. Can this situation be described somehow using a quantum mechanical state? Well, unless we happen to have $|a\rangle = |b\rangle$ there is no state vector that will give a satisfactory description of this, and so the situation can not be described by a 'pure' state. This is why we introduce what is called mixed states, which are described by state operators or density operators instead of state vectors.

Density operators are a more general description of quantum mechanical states, since these can be used to describe both pure and mixed states. In the case of a pure state there must obviously be some connection between the state operator and the state vector descriptions. Let us begin by explaining this: If the state vector of a system is $|\psi\rangle$, then the state operator is simply $\rho = |\psi\rangle\langle\psi|$. Now, remember that in the pure state formalism the probability of finding the system in some state $|\phi\rangle$ in a measurement is given by $p = |\langle\phi|\psi\rangle|^2$. This can be rephrased as $p = \langle\phi|\psi\rangle\langle\psi|\phi\rangle = \langle\phi|\rho|\phi\rangle$, which is the general formula for such probabilities in the state operator formalism.

Given this, it is easy to see that this formalism can be generalized to situations such as the one above, where the system is in the pure states $|a\rangle$ or $|b\rangle$, each with a probability of 1/2. The state operator describing this 'mixed' state is simply $\rho = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b|$. We can see this by applying the mentioned probability formula to this operator. According to this formula, the probability of finding the system in the pure state $|\phi\rangle$ in a measurement is $\langle\phi|\rho|\phi\rangle = \frac{1}{2}|\langle\phi|a\rangle|^2 + \frac{1}{2}|\langle\phi|b\rangle|^2$, which is precisely what it should be. In general, if a system is prepared in pure states $|i\rangle$ with probability p_i, the state operator will be

$$\rho = \sum_i p_i |i\rangle\langle i| , \tag{2.1}$$

It is clear that a state operator must always satisfy two particular conditions. First, it must be a positive operator. That is, for any state vector $|\psi\rangle$ we must have $\langle\psi|\,\rho\,|\psi\rangle \geq 0$. The reason for this, is that this is the general probability formula, and any probability must be larger than zero. Secondly, the operator must have trace 1. That is, it must satisfy the relation

$$\operatorname{Tr}\rho = \sum_i \langle i|\,\rho\,|i\rangle = 1, \tag{2.2}$$

where $|i\rangle$ forms a orthonormal basis of the involved Hilbert space. The reason for this is that such a basis forms all the possible outcomes of a particular measurement, and so their probabilities must sum to 1. Any operator that satisfies these two requirements is in fact a valid state operator. It can always be written either in the form 2.1 or as a similar expression involving an integral.

In particular, if the state operator describes a thermal state, then it may be written as

$$\rho = \sum_i p_i\,|E_i\rangle\,\langle E_i|\,, \tag{2.3}$$

where the set $\{|E_i\rangle\}$ is a basis of energy eigenvectors with E_i the corresponding eigen values, and the probabilities p_i are proportional to the Boltzmann factors $e^{-\beta E_i t}$. Here β is related to the temperature of the thermal state through the definition $\beta = \frac{1}{k_B T}$, where k_B is Boltzmann's constant and T is the temperature. It is easily seen that 2.3 can be expressed simply as

$$\rho = \frac{1}{Z}e^{-\beta H}, \tag{2.4}$$

where H is the systems Hamiltonian and Z is a normalization factor which is known as the partition function. From 2.2 we see that

$$Z(\beta) = \operatorname{Tr} e^{-\beta H}. \tag{2.5}$$

2.1.1 The fundamental postulates

The fundamental postulates of quantum mechanics are usually formulated using state vectors, but it is fully possible to reformulate these completely in terms of the density operator formalism. I will do this here, since it will give the reader an increased understanding of the formalism and because it is this formulation that will form our starting point when we wish to generalize the quantum mechanical theory to open systems. Note that all of the following postulates can be derived from the standard formulation using the rules and definitions above.

Postulate 1: Quantum mechanical states. The state of a quantum mechanical system is described by a positively definite density operator ρ with trace 1.

Postulate 2: Measurable quantities. Any measurable quantity a of a quantum systems is associated to a Hermitian operator A. The only possible outcomes of a measurement of this quantity are the eigenvalues of A. The operator A can be written as either a sum or an integral of terms of type $a'P'$, where a' is an eigen value, and P' the projection operator onto the corresponding eigenspace. This projection operator is associated to the proposition 'Measurement of a gives result a'' (see Postulate 3).

Postulate 3: Probabilities. Any proposition q about measurements on a quantum system is associated to a projection operator $P_q = P_q^2$. The probability of the proposition q being true in a concrete measurement is given by $p_q = \operatorname{Tr} P_q\rho$. In the event that the proposition q corresponds to a single pure state $|q\rangle$, this expression becomes $p_q = \langle q|\,\rho\,|q\rangle$.

Postulate 4: Expectation values. If a measurable quantity a is associated to the Hermitian operator A, then the expectation value of the quantity a in a concrete measurement is given by $\langle a\rangle = \operatorname{Tr} A\rho$.

Postulate 5: Time development (in the Schrödinger picture). The time development of a quantum mechanical system is described by a unitary time development operator $U(t)$. If the initial state of the system is described by the density operator $\rho(0)$, then the state at time t will be $\rho(t) = U(t)\rho(0)U(t)^\dagger$. Since $U(t)$ is normally assumed to be differentiable, we may define the Hamiltonian operator $H(t)$ as $H(t) = \hbar i \dot{U}(t)U(t)^\dagger$. The state operator $\rho(t)$ then satisfies the quantum mechanical Liouville equation $\dot{\rho} = -\frac{i}{\hbar}[H, \rho]$.

Postulate 6: The collapse postulate. Immediately after a measurement is performed the quantum mechanical state goes through an instantaneous and irreversible change referred to as a 'collapse'. In the density operator formalism the state after the collapse depends on whether the result of the measurement is read or discarded. If it is discarded the new state will be $\rho' = \sum_i P_i \rho P_i$, where P_i are the projection operators corresponding to all the possible measurement results. If the measurement result is read, then the new state will be $\rho' = P_m \rho P_m / \mathrm{Tr}\, P_m \rho$, where P_m is the projection operator corresponding to the actual result.

for a more comprehensive discussion of the density operator formalism, see for instance [7] or [1].

2.2 Quantum mechanics of composite systems

2.2.1 Tensor products and tensor product spaces

Going back to the pure state formalism now for a while, let us assume that we have two quantum systems A and B. The pure states of A are described by vectors in a Hilbert space $\mathcal{H}_A$, while the pure states of B are described by vectors in a Hilbert space $\mathcal{H}_B$. But what about the pure states of the composite system $C = A \cup B$? What Hilbert space do they form? The answer is that they form the *tensor product space* $\mathcal{H}_C = \mathcal{H}_A \otimes \mathcal{H}_B$.

The tensor product space is a new Hilbert space which is defined more or less through the requirement that if $\{|a\rangle : a \in \mathcal{A}\}$ is a basis of $\mathcal{H}_A$ and $\{|b\rangle : b \in \mathcal{B}\}$ is a basis of $\mathcal{H}_B$, then $\{|a\rangle \otimes |b\rangle : a \in \mathcal{A}, b \in \mathcal{B}\}$ forms a basis for $\mathcal{H}_A \otimes \mathcal{H}_B$. In this definition we have also introduced the tensor product between two vectors: Given a vector $|a\rangle$ in $\mathcal{H}_A$ and a vector $|b\rangle$ in $\mathcal{H}_B$, the tensor product $|a\rangle \otimes |b\rangle$ is a vector in the tensor product space $\mathcal{H}_A \otimes \mathcal{H}_B$. The tensor product is bilinear, meaning that

$$(e\,|a\rangle) \otimes |b\rangle = |a\rangle \otimes (e\,|b\rangle) = e\,|a\rangle \otimes |b\rangle\,, \tag{2.6}$$

$$(|a\rangle + |c\rangle) \otimes |b\rangle = |a\rangle \otimes |b\rangle + |c\rangle \otimes |b\rangle \text{ and} \tag{2.7}$$

$$|a\rangle \otimes (|b\rangle + |d\rangle) = |a\rangle \otimes |b\rangle + |a\rangle \otimes |d\rangle\,. \tag{2.8}$$

We may define the inner product of vectors in the tensor product space through the simple relation $(\langle a'| \otimes \langle b'|)(|a\rangle \otimes |b\rangle) = \langle a'|a\rangle\langle b'|b\rangle$. Here $\langle a'| \otimes \langle b'|$ should be interpreted simply as the dual vector of $|a'\rangle \otimes |b'\rangle$. We may also define the tensor product of two operators acting on $\mathcal{H}_A$ and $\mathcal{H}_B$ through the relation $(A \otimes B)\,|a\rangle \otimes |b\rangle = A\,|a\rangle \otimes B\,|b\rangle$. Note that linearity makes this an unambiguous definition of $A \otimes B$, and that all operators acting on $\mathcal{H}_A \otimes \mathcal{H}_B$ may be written as a sum of operators in this 'tensor product form'.

When working with tensor product spaces it is often useful to extend the algebra of operators, bras and kets a little bit. For instance, if $|a'\rangle$ is a vector in $\mathcal{H}_A$, then it is sometimes useful to define the action of $\langle a'|$ on vectors in $\mathcal{H}_A \otimes \mathcal{H}_B$. This can be done through the relation $\langle a'|\,(|a\rangle \otimes |b\rangle) = \langle a'|a\rangle \cdot |b\rangle$, which again is an unambiguous definition due to linearity. Several relations like this are shown in the list below, where it is assumed that $|a\rangle$ and $|a'\rangle$ are vectors in $\mathcal{H}_A$, $|b\rangle$ and $|b'\rangle$ are vectors in $\mathcal{H}_B$ and that A and B

are operators acting on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively:

$$\langle a'| (|a\rangle \otimes |b\rangle) = \langle a'|a\rangle |b\rangle , \tag{2.9}$$

$$\langle b'| (|a\rangle \otimes |b\rangle) = \langle b'|b\rangle |a\rangle , \tag{2.10}$$

$$(\langle a'| \otimes \langle b'|) |a\rangle = \langle a'|a\rangle \langle b'| , \tag{2.11}$$

$$(\langle a'| \otimes \langle b'|) |b\rangle = \langle b'|b\rangle \langle a'| , \tag{2.12}$$

$$A(|a\rangle \otimes |b\rangle) = A|a\rangle \otimes |b\rangle , \tag{2.13}$$

$$B(|a\rangle \otimes |b\rangle) = |a\rangle \otimes B|b\rangle , \tag{2.14}$$

$$(\langle a'| \otimes \langle b'|)A = \langle a'| A \otimes \langle b'| , \tag{2.15}$$

$$(\langle a'| \otimes \langle b'|)B = \langle a'| \otimes \langle b'| B, \tag{2.16}$$

$$\langle a'| (A \otimes B) |a\rangle = \langle a'| A |a\rangle B, \tag{2.17}$$

$$\langle b'| (A \otimes B) |b\rangle = \langle b'| B |b\rangle A. \tag{2.18}$$

For an extended discussion of tensor products and tensor product spaces, see [1].

2.2.2 Partial traces and reduced density operators.

Remember that the trace of an operator O acting on a Hilbert space $\mathcal{H}$ is defined as

$$\mathrm{Tr}\, O = \sum_i \langle i| O |i\rangle , \tag{2.19}$$

where $\{|i\rangle\}$ forms an orthonormal basis of $\mathcal{H}$. If O actually acts on the tensor product space $\mathcal{H}_A \otimes \mathcal{H}_B$, then taking into account the lower most definitions of 2.9 we may define the *partial traces* of O as the operators given by

$$\mathrm{Tr}_A\, O = \sum_a \langle a| O |a\rangle \text{ and} \tag{2.20}$$

$$\mathrm{Tr}_B\, O = \sum_b \langle b| O |b\rangle , \tag{2.21}$$

where $\{|a\rangle\}$ and $\{|b\rangle\}$ are assumed to form orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively. Note that the definition 2.20 clearly implies that

$$\mathrm{Tr}\, O = \mathrm{Tr}\, \mathrm{Tr}_A\, O = \mathrm{Tr}\, \mathrm{Tr}_B\, O. \tag{2.22}$$

In addition to this, the following simple demonstration shows that a partial trace of a possitive operator will itself be positive:

$$\langle \psi| \mathrm{Tr}_A \rho |\psi\rangle = \sum_a (\langle a| \otimes \langle \psi|)\rho(|a\rangle \otimes |\psi\rangle \geq 0. \tag{2.23}$$

These relations means that if we have a density operator ρ_C of the composite system $C = A \cup B$ (that is, an operator acting on $\mathcal{H}_C = \mathcal{H}_A \otimes \mathcal{H}_B$ that has trace 1 and is positively definite), then we get new density operators by taking the partial traces of ρ_C. These are referred to as the *reduced density operators*, *reduced state operators* or just *reduced states* of the systems A and B. To write things out explicitly, the reduced state ρ_A of A and the reduced state ρ_B of B are defined as

$$\rho_A = \mathrm{Tr}_B\, \rho_C, \tag{2.24}$$

$$\rho_B = \mathrm{Tr}_A\, \rho_C. \tag{2.25}$$

Take note that these operators are indeed acting on the correct Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively.

So what is the significance of the reduced states ρ_A and ρ_B? Well, it turns out that if one is really only interested in for instance the properties of system A, then all of these are in fact *completely* described by the reduced state ρ_A. Obviously it is the same way if one is only interested in system B. Note that something similar does not exist in the pure state formalism: Given some pure state $|\psi\rangle$ in $\mathcal{H}_A \otimes \mathcal{H}_B$, there is in general no single pure state $|a\rangle$ in $\mathcal{H}_A$ that shares all the properties of A with $|\psi\rangle$.

As for ρ_C and ρ_A however, this is in fact the case. We may show this by proving that any proposition q about A has the same probability for being true given the state ρ_A as the state ρ_C. Using Postulate 3 from above, this is easily done:

$$\begin{aligned} p_q =& \mathrm{Tr} P_q \rho_A = \mathrm{Tr} P_q \mathrm{Tr}_B \rho_C \\ =& \mathrm{Tr} \sum_b P_q \langle b| \rho_C |b\rangle = \mathrm{Tr} \sum_b \langle b| P_q \rho_C |b\rangle \\ =& \mathrm{Tr}\mathrm{Tr}_B P_q \rho_C = \mathrm{Tr} P_q \rho_C = p_q. \end{aligned} \tag{2.26}$$

Here P_q acts only on $\mathcal{H}_A$ since q is a proposition about A. In the theory open systems, where the quantum system S of interest is coupled to an environment E that we are not really interested in, this result is obviously very useful. In fact this is the main reason why the density operator formalism is so important in the theory of open systems.

For a more general discussion of the properties of reduced states, the reader is again referred to [7] or [1].

2.3 The two level system and Harmonic oscillator

In this final section of the prerequisites chapter, I will give a very rapid review of the description of two central quantum mechanical models: the two level system and harmonic oscillator. This is because these will be the two models I will use for illustration of the theory in the main text. There, the two systems will obviously be regarded as open systems, whereas in this review they are simply the standard closed system models. These models are studies in as good as all texts on quantum mechanics, such as [5][1][7].

2.3.1 The two level system

The two level system is just like the name suggests simply a system with two, and only two, distinct states. These states are often, but not always, assumed to have different energy. They then form two different energy levels, which is the origin of the name. The Hilbert space of this model is simply a standard two dimensional vector space with an inner product. Low dimensional systems like this are typically described using the matrix representation, where the kets are represented as column vectors, the bras as row vectors and the operators as square matrices. In this case all of these have dimension two.

The vectors corresponding to the two states form an orthonormal basis for the Hilbert space. These two states are often denoted $|1\rangle$ and $|2\rangle$, $|\downarrow\rangle$ and $|\uparrow\rangle$, $|g\rangle$ and $|e\rangle$ or something similar. In the matrix representation they are typically written as

$$|1\rangle = |\downarrow\rangle = |g\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \text{ and} \tag{2.27}$$

$$|2\rangle = |\uparrow\rangle = |e\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.28}$$

In addition to this there exists a standard notation for certain operators acting on these states, or more precisely on the associated Hilbert space spanned out by them. In the matrix representation, the

standard nomenclature is

$$P_e = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |e\rangle\langle e|, \tag{2.29}$$

$$P_g = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = |g\rangle\langle g|, \tag{2.30}$$

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{2.31}$$

$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{2.32}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_+ + \sigma_-, \tag{2.33}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i\sigma_+ + i\sigma_-, \text{ and} \tag{2.34}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.35}$$

The matrices σ_x, σ_y and σ_z are frequently denoted the Pauli matrices. One particular system that may be described by this model is a spin half system, where these matrices are connected respectively to the x, y and z components of the angular momentum.

Typically, the Hamiltonian of the system is taken to be proportional to σ_z, as in for instance $H = \Delta\sigma_z$, which would describe a system with two energy levels separated by 2Δ. If the Hamiltonian has terms that are proportional to σ_x or σ_y, then the states $|e\rangle$ and $|g\rangle$ are not energy eigenstates.

2.3.2 The Harmonic oscillator and the coherent state representation

The Harmonic oscillator is a system described by a Hamiltonian of type

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2, \tag{2.36}$$

where x and p are operators satisfying the canonical commutation relations $[x, p] = \hbar i$. In classical mechanics this Hamiltonian describes a system that follows the equation $\ddot{x} = -\omega^2 x$, and thus undergoes simple oscillatory motion. An example could for instance be a mass in a spring. The reader should already be familiar with this.

In quantum mechanics, a Hamiltonian of this form leads to a system with a discrete but infinite number of energy levels. The system has a lowest energy level (a ground state), but no highest. The spacing between the levels is constant and equal to $\hbar\omega$. The ground state has energy $\hbar\omega/2$. Due to this regularity, one may define the so called number operator $N = H/\hbar\omega - \frac{1}{2}$. This operator has integer eigenvalues n in the range from 0 to infinity, and it counts the number of excitations of the oscillator, or equivalently how many energy levels it is currently above the ground state. The energy of this state may be found through the formula $E = \hbar\omega(n + 1/2)$. The harmonic oscillator Hamiltonian is sometimes simply written as $H = \hbar\omega N$, where the ground state energy is omitted.

If this representation of the Hamiltonian is used, then the thermal states of the oscillator will be given by the expression

$$\rho = \frac{1}{Z}e^{-\beta\hbar\omega N}. \tag{2.37}$$

From 2.5 we see that the partition function Z is simply

$$Z(\beta) = \sum_n e^{-\beta\hbar\omega n} = \frac{1}{1 - e^{-\beta\hbar\omega}}, \tag{2.38}$$

so that in fact

$$\rho = (1 - e^{-\beta\hbar\omega})e^{-\beta\hbar\omega N}. \tag{2.39}$$

The number operator may also be written as $N = a^\dagger a$, where a and $a^\dagger$ are adjoint operators known as the annihilation and creation operator. These operators may be defined in terms of the canonical operators x and p through the formulas

$$a = \frac{m\omega x + ip}{\sqrt{2m\hbar\omega}} \tag{2.40}$$

$$a^\dagger = \frac{m\omega x - ip}{\sqrt{2m\hbar\omega}} \tag{2.41}$$

[5]. From this it can be shown that they satisfy the commutation relation $[a, a^\dagger] = 1$. The annihilation operator a lowers the energy by one level, or equivalently it annihilates one excitation. The creation operator $a^\dagger$ increases the energy by one level, or equivalently it creates one excitation[5]. Note that if the oscillator is actually a mode in some bosonic quantum field, then these excitations are in fact particles.

The annihilation operator a also has eigenvectors and eigenvalues. Unlike the eigenvalues of N however, the ones of a are complex and form a continuum instead of a discrete set. These eigenvectors are known as coherent states. A common way to represent these states is to introduce the unitary *displacement operator*

$$D(z) = e^{za^\dagger - z^\star a} = e^{-\frac{1}{2}|z|^2} e^{za^\dagger} e^{-z^\star a}, \tag{2.42}$$

where we have employed the so called Bacer-Cambell-Hausdorf formula, which states that if two operators A and B satisfies the relations $[A,[A,B]] = [B,[A,B]] = 0$, then $e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$.

Using this operator we may define the coherent state $|z\rangle$ as

$$|z\rangle = D(z)\,|0\rangle\,, \tag{2.43}$$

where $|0\rangle$ is the ground state (frequently denoted the *vacuum*). It can be shown that the displacement operators $D(z)$ satisfies the relation

$$D(z)^\dagger a D(z) = a + z \tag{2.44}$$

[7]. In particular this means that

$$a\,|z\rangle = aD(z)\,|0\rangle = D(z)(a+z)\,|0\rangle = zD(z)\,|0\rangle = z\,|z\rangle\,, \tag{2.45}$$

which demonstrates that the coherent states are indeed eigenvectors of the annihilation operator a, and that the eigenvalue is z.

It should be noted that two coherent states are not orthogonal. In fact, it can be shown[7] that the overlap between a coherent state and an eigenvector $|n\rangle$ of the number operator is

$$\langle n|z\rangle = \frac{z^n}{\sqrt{n!}} e^{-\frac{1}{2}|z|^2}, \tag{2.46}$$

and accordingly the overlap between two coherent states $|z\rangle$ and $|w\rangle$ is

$$\langle w|z\rangle = \langle w| \sum_n |n\rangle\,\langle n|\,|z\rangle = \sum_n \frac{w^{\star n} z^n}{n!} e^{-\frac{1}{2}|z|^2} e^{-\frac{1}{2}|w|^2} = e^{-\frac{1}{2}|z|^2 + w^\star z - \frac{1}{2}|w|^2}. \tag{2.47}$$

Even though the coherent states are not orthogonal they still form a basis for the Hilbert space of the oscillator. This basis is however overcomplete, in the sense that vectors may not be expanded in this basis in a unique way. While the identity relation of orthogonal bases like for instance momentum states satisfies identity relations of type

$$\int_{-\infty}^{\infty} dp \, |p\rangle \langle p| = I, \tag{2.48}$$

the coherent states instead satisfies the relation

$$\int_{\mathbb{C}} d^2 z \, |z\rangle \langle z| = \pi \tag{2.49}$$

[7]. In particular this means that one of the (non unique) ways of expressing a general state $|\psi\rangle$ as a linear combination of coherent states, is through the formula

$$|\psi\rangle = \int_{\mathbb{C}} \frac{d^2 z}{\pi} \, |z\rangle \langle z|\psi\rangle, \tag{2.50}$$

which is known as the coherent state representation[7].

Part I

The general theory of open systems

Chapter 3

Introduction to open quantum systems

3.1 Time development in open systems

In section 2.1.1 we saw the fundamental postulates of quantum mechanics written in terms of density operator formalism. However, this formulation just like any other assumes the system under study to be *closed*. That is, it assumes that as opposed to an *open system*, it does not interact with its surroundings. To be more precise, this is assumed in the 5. postulate which discusses time development. There is no reason to assume that the remaining postulates would in any way be affected by interactions with an environment, but the 5. postulate would be strongly affected by this: In open systems the unitarity of time development will in general break down, as I shall soon demonstrate.

Given then that the time development postulate is really limited to closed systems, one might wonder whether one can at all justify using this to describe systems in the real world. After all, apart from perhaps the universe in its totality, no system is truly closed in this sense. Thus, the assumption must always be an approximation only. Quite often however, it will be a very good approximation. The reason for this is that in many cases the interactions with the environment are very weak, and they induce significant changes in the system only after times that are much longer than the duration of a typical experiment. There will however obviously also be cases where this is not true. That is, where the interactions with the environment are so strong, or alternatively the experiment is carried out over such a long time that it will be significantly affected by these interactions. In such cases one must take explicitly in account the open nature of the system.

Such open systems is the subject of this thesis, and especially their time development. One might say that the central question to be treated, is what we are to replace the time development postulate with when we are dealing with open systems. Other connected subjects to be treated are the characteristics of the time development of open systems and how this differs from closed systems, together with a discussion of the methods one might use to find this development.

But first we should go into some more detail of what is meant by an open system, and how we are to describe these. As mentioned an open system is a system that is interacting with its surrounding environment. In a real physical system this surrounding environment would simply be the rest of the world. To be more precise about this description, we denote the the system S, and we say that it is coupled to an environment E. The system S together with its environment forms the total system T. As explained in section 2.2.1, T will have a corresponding Hilbert space $\mathcal{H}_T = \mathcal{H}_T \otimes \mathcal{H}_E$, where $\mathcal{H}_S$ is the Hilbert space of S and $\mathcal{H}_E$ is the Hilbert space of E. We treat the total system $T = S \cup E$ as being closed. This allows us to assume that it evolves unitarily as described by the standard time development postulate.

In this part, where we discuss the general properties of open systems, the justification for treating T as closed is simply that we take E to be the entire rest of the world. This means that T will in fact be the entire universe, and thus a closed system. If not a certainty this is at least a very very natural assumption. However, in an actual application of this idea, where we perhaps wish to derive a description of S from a description of T in some way, the same justification does not work equally well. In such a

case, where we would need a concrete model of E we could not let this be the entire rest of the world: At the present time we are sadly not so fortunate as to know either the state nor the Hamilton operator of the entire universe. And even if we did, it would surely not be possible to take all of this information into account in any meaningful way.

In fact, in practical calculations we can really only include the most immediate environment of S in our model of E. Thus we will need another justification for treating $S \cup E$ as closed, which is what I will attempt to provide in the following: In realistic situations the immediate environment E of S must be assumed to be a macroscopic system in a state which will usually be thermal. As long as E is sufficiently large and in equilibrium with the rest of the world (R), the interactions with R can only produce small perturbations in the state of E. In order for such small perturbations to have any significant effect on S, they would have to be correlated with it in some way. Such correlations are highly unlikely to exist unless they are made by intent. If such intent exists, then it must obviously be included in the model of either S or E.

To exemplify this, consider an atom A in an exited state. This atom will be coupled to the electromagnetic field, and so given sufficient time it must emit a photon and fall into its ground state. In a model capable of reproducing this behavior we must obviously include the electromagnetic field, but what about other objects? This could for instance be additional atoms which are not themselves coupled to A, but are coupled to the electromagnetic field. Must they also be included in the model? After all these extra atoms could scatter the photon in such a way that it is sent back to A and re-excites it.

Well, if they are very close to A, then the atoms must be considered part of As immediate environment, and so they must be included if high accuracy is required. If they are distant, then the scattered parts of the photon will have an incredibly small amplitude when returning to A, and the effect on the state will be negligible. That is, the probability of excitement will be vanishingly small. If however the extra atoms are arranged in a particular way, such as for instance forming a spherical mirror with its center in A, then the entire photon would return to A at the same time, and re-excitement would be as good as certain.

The photon, which is a small perturbation of the electromagnetic field, would then be correlated with A and the origin of this correlation, the mirror, would have to be included in the model. Note that any such configuration of atoms is extremely unlikely to exist unless it has actually been placed there by an experimentalist. That is, it is made by intent, so that whether it is to be included in the model or not becomes a rather stupid question.

Having now justified the treatment of the total system T as closed, we may return to our discussion of the properties of the open system S. Seeking as we do to find some general description of the time development of this, we may take to our advantage the assumption that T develops unitarily. In fact, we can even use this to find an exact expression for this development: Let $\rho_T(0)$ be the initial state operator of the full system T. Let $U(t)$ be the time development operator of T. Then from the 5. postulate of 2.1.1 the state of the full system at time t will be $\rho_T(t) = U(t)\rho_T(0)U^\dagger(t)$. From 2.24 and the belonging discussion we see that the reduced state of the system S can be found through the formula $\rho_S = \mathrm{Tr}_E\rho_T$. This means that the state of ρ_S at time t will in fact be

$$\rho_S(t) = \mathrm{Tr}_E(U(t)\rho_T(0)U^\dagger(t)), \tag{3.1}$$

which is the most general description of the time development of an open quantum system. There is however one problem with this expression. This is that the involved operators $U(t)$ and $\rho_T(0)$ belong to the total system T. I will soon explain why this is problematic, but first I will use 3.1 to demonstrate an earlier assertion: namely that the the development of the reduced system S will in general not be unitary.

To do this, we keep in mind that a unitary development will turn pure states into pure states: Any pure state $|\psi\rangle$ is taken to a new pure state $U(t)|\psi\rangle$. Thus, all we need to do to demonstrate that 3.1 does not in general describe a unitary development of $\rho_S(t)$, is to show that this development may take a pure state at $t = 0$ to a mixed state at a later time. This is easy to do by a simple example: Let the system S consist of a simple two level system having the two states $|\uparrow\rangle$ and $|\downarrow\rangle$. Let also the environment E be described simply by a system of the same type. The total system T will then have four tensor product states, which are named $|\uparrow\uparrow\rangle$, $|\downarrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$ and $|\downarrow\downarrow\rangle$ in the obvious fashion.

We now assume that at some particular time t the unitary time development operator $U(t)$ takes the state $|\uparrow\uparrow\rangle$ to the new state $(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$. Expressed using density operators this means that if $\rho_T(0) = |\uparrow\uparrow\rangle\langle\uparrow\uparrow|$, then $\rho_T(0) = U(t)\rho_T(0)U^\dagger(t) = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)(\langle\uparrow\uparrow| + \langle\downarrow\downarrow|)/2$. It is now easy to see that $\rho_S(0) = \mathrm{Tr}_E\rho_T(0) = |\uparrow\rangle\langle\uparrow|$ which is a pure state, while $\rho_S(t) = \mathrm{Tr}_E\rho_T(t) = (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)/2$ which is a mixed state. Thus the time development of S can not be unitary.

Even so, one of the simplest ways of dealing with environmental effects is to make a modification of the Hamiltonian, and thus keep the unitary development. As demonstrated above such a model would not be able to account for all the effects of openness. But as long as what one might call the unitary contribution from the environment is the most important one, the model could be expected to work quite well. A typical modification one could make is to add to the Hamiltonian H_S of S the term $\mathrm{Tr}_E(H_{SE}\rho_E(t))$, with H_{SE} being the interaction part of the Hamiltonian of the full system $S \cup E$, and $\rho_E(t)$ being a time dependent state of the environment.

Doing this corresponds essentially to assuming that although the environment may have a strong effect on S, it is not in any significant way affected back in return. In other words we are in a way assuming the environment to be a 'classical' system. The modification above is in fact precisely what one does whenever one creates a model where the quantum system is being affected by some classical background. This classical background could for instance be an electromagnetic field of some sort. In this case $\mathrm{Tr}_E(H_{SE}\rho_E(t))$ would simply be H_{SE}, but with the electromagnetic field operator replaced by its average. Making this kind of approximation is typically denoted semiclassical theory.[5]

In this Thesis we will however go beyond semiclassical approximations like this. We are interested in more realistic ways to model open systems, and so using unitary models is not an option. As mentioned above, the most realistic and most general model is 3.1. So why can we not simply apply this directly? Well, in some very simple cases we can. We shall see examples of this later, as this will be applied to both of my two example models. Nevertheless, it is important to realize that the direct application of 3.1 is limited to very simple models of the environment E, and very simple models of the interactions between E and S. The application of this formula involves solving the Shrödinger equation for the full system T, which in realistic models would be impossible due to this system having a macroscopic number of degrees of freedom. In addition to this, the partial trace in 3.1 might also be a quite messy calculation, as will be seen in the chapter on the open harmonic oscillator.

What one is really interested in then, is some method that reproduces (or at least approximates) the behavior of ρ_S without taking the degrees of freedom of E explicitly into account. In a sense what we want is a generalization of the standard time development postulate $\rho(t) = U(t)\rho(0)U^\dagger(t)$, and preferably a generalization also of the Shrödinger or Liouville equations. We will return to the question of a generalized Shrödinger equation later, but for now let us concentrate on whether we can generalize the unitary time development formula. One possible such generalization is known as the Kraus decomposition and will be treated in the next section. There it will be demonstrated that the exact development of $\rho(t)$ can be written in such a Kraus form, provided that we make one additional assumption:

In 3.1, the initial state of the full system T is completely general, so that the system S may have both classical and quantum mechanical correlations with the environment. To get the expression on Kraus form we will assume instead that there are no correlations of any type at $t = 0$. That is we assume that the initial state factorizes as $\rho_T(0) = \rho_S(0) \otimes \rho_E(0)$. This will turn 3.1 into

$$\rho_S(t) = \mathrm{Tr}_E(U(t)(\rho_S(0) \otimes \rho_E(0))U^\dagger(t)), \tag{3.2}$$

which, if $\rho_E(0)$ is regarded as fixed, expresses $\rho_S(t)$ in terms of $\rho_S(0)$ alone. This is of course a necessity to construct a meaningful generalization of the formula $\rho(t) = U(t)\rho(0)U^\dagger(t)$. Another way of thinking of this is that 3.2 defines a map taking $\rho_S(0)$ to $\rho_S(t)$. Since in this case the map is actually linear, it can be thought of as an operator $\mathcal{G}_t$ acting on the space of state operators. Such an operator acting on other operators is often referred to as a *super operator*.

At first glance the assumption of factorizing initial conditions might seem to greatly reduce the generality of our treatment. We would after all expect interactions with the environment to cause any open system to form correlations with this. However, the situation is actually not as bad as it seems. As long as

the interactions are relatively weak, then so will typically also the correlations be. Thus, the consequences of ignoring these will not be all that dramatic. In this thesis we shall almost always assume factorizing initial conditions. Even so, some of the methods to be discussed can be generalized to descriptions that does not assume this condition, and in particular there are good reasons to believe that the Kraus form holds more generally. This will be discussed in more detail in the next section.

3.2 Kraus Decomposition

To get 3.2 in the form known as Kraus decomposition[1], we begin by diagonalizing $\rho_E(0)$ and $\rho_S(0)$ to get

$$\rho_E(0) = \sum_i p_i \left|i\right\rangle \left\langle i\right|, \tag{3.3}$$

$$\rho_S(0) = \sum_k q_k \left|k\right\rangle \left\langle k\right|, \tag{3.4}$$

with $\{|i\rangle\}$ an orthonormal basis for $\mathcal{H}_E$ consisting of eigenvectors of $\rho_E(0)$, and $\{|k\rangle\}$ an orthonormal basis for $\mathcal{H}_S$ consisting of eigenvectors of $\rho_S(0)$. Then, we define the operators $U_{ij}(t)$ on $\mathcal{H}_S$ by

$$U_{ij}(t) = \left\langle i\right| U(t) \left|j\right\rangle, \tag{3.5}$$

with $|i\rangle$ and $|j\rangle$ from the eigenvector basis $\{|i\rangle\}$. We can then write 3.2 as

$$\begin{aligned}\rho_S(t) &= \sum_i \left\langle i\right| \left(U(t)(\rho_S(0)\otimes\rho_E(0))U^\dagger(t)\right) \left|i\right\rangle = \sum_{ij} p_j \left\langle i\right| U(t)(\rho_S(0)\otimes \left|j\right\rangle \left\langle j\right|)U^\dagger(t) \left|i\right\rangle \\ &= \sum_{ijk} p_j q_k \left\langle i\right| U(t)(\left|k\right\rangle \left\langle k\right| \otimes \left|j\right\rangle \left\langle j\right|)U^\dagger(t) \left|i\right\rangle = \sum_{ijk} p_j q_k (\left\langle i\right| U(t) \left|k\right\rangle \otimes \left|j\right\rangle)(\left\langle k\right| \otimes \left\langle j\right| U^\dagger(t) \left|i\right\rangle) \\ &= \sum_{ijk} p_j q_k U_{ij}(t) \left|k\right\rangle \left\langle k\right| U_{ij}^\dagger(t) = \sum_{ij} p_j U_{ij}(t)\rho_S(0)U_{ij}^\dagger(t).\end{aligned} \tag{3.6}$$

Further defining $V_{ij} = \sqrt{p_j}U_{ij}$ we will get

$$\rho_S(t) = \sum_{ij} V_{ij}(t)\rho_S(0)V_{ij}^\dagger(t). \tag{3.7}$$

The operators V_{ij} also satisfy the relation

$$\begin{aligned}\sum_{ij} V_{ij}^\dagger V_{ij} &= \sum_j p_j \sum_{ik} U_{ij}^\dagger \left|k\right\rangle \left\langle k\right| U_{ij} = \sum_j p_j \sum_{ik} \left\langle j\right| U^\dagger(\left|k\right\rangle \left\langle k\right| \otimes \left|i\right\rangle \left\langle i\right|)U \left|j\right\rangle \\ &= \sum_j p_j \left\langle j\right| U^\dagger U \left|j\right\rangle = \sum_j p_j \left\langle j\right| I_T \left|j\right\rangle = \sum_j p_j I_S = I_S,\end{aligned} \tag{3.8}$$

with I_T the identity operator on $\mathcal{H}_T$ and I_S the identity operator on $\mathcal{H}_S$. Now simply re-indexing our V operators, we get the Kraus form of the time development:

$$\rho_S(t) = \sum_i V_i(t)\rho_S(0)V_i^\dagger(t), \text{ with} \tag{3.9}$$

$$\sum_i V_i^\dagger(t)V_i(t) = I. \tag{3.10}$$

Note that if we limit the number of V operators to one, we recover the old unitary time development of closed systems so that unitary development is in fact a special case of the Kraus decomposition.

3.9 can however also describe processes that does not conserve the purity of states, and thus it is more general. Also, as I have already mentioned, even though the derivation above was given under the assumption that the initial state factorizes there are reasons to believe that 3.9 is more general. This is because given certain conditions this expression is actually the most general expression one can have for the time development of a state operator. Aspects of these conditions will be discussed in the next section, but first we will state and prove the full theorem of Kraus Decomposition.

Theorem 1. Kraus Decomposition.

Let $L(\mathcal{H})$ be the space of linear operators A on a Hilbert space $\mathcal{H}$. Let $\mathcal{L} : L(\mathcal{H}) \to L(\mathcal{H})$ be a map from $L(\mathcal{H})$ to itself. Then $\mathcal{L}$ can be written in Kraus form:

$$\mathcal{L}(A) = \sum_i V_i A V_i^\dagger, \text{ with} \tag{3.11}$$

$$\sum_i V_i^\dagger V_i = I, \tag{3.12}$$

if and only if the following conditions are satisfied:

(a) $\mathcal{L}$ is linear. That is, $\mathcal{L}$ is a super operator acting on $L(\mathcal{H})$.

(b) $\mathcal{L}$ is trace preserving.

(c) $\mathcal{L}$ is completely positive, meaning that given any additional Hilbert space $\mathcal{H}_2$, the linear map $\mathcal{L} \otimes I : L(\mathcal{H} \otimes \mathcal{H}_2) \to L(\mathcal{H} \otimes \mathcal{H}_2)$ is positive.

Proof. The proof is based on one that is found in [2]. A similar proof can also be found in [10]. Let us first verify that a map in Kraus form satisfies the conditions above. The condition of linearity is obviously satisfied, and to check the second condition we do the following simple calculation:

$$\mathrm{Tr}\left(\sum_i V_i A V_i^\dagger\right) = \sum_i \mathrm{Tr} A V_i^\dagger V_i = \mathrm{Tr} A \sum_i V_i^\dagger V_i = \mathrm{Tr} A. \tag{3.13}$$

The final condition is also easily verified by first noting that the map $\mathcal{L} \otimes I$ can be written as

$$\begin{aligned}(\mathcal{L} \otimes I)A' =& (\mathcal{L} \otimes I) \sum_j A_j \otimes A_{2j} = \sum_j (\mathcal{L} A_j) \otimes A_{2j} = \sum_{ij} (V_i A_j V_i^\dagger) \otimes A_{2j} \\ =& \sum_{ij} (V_i \otimes I)(A_j \otimes A_{2j})(V_i \otimes I)^\dagger = \sum_i (V_i \otimes I) A' (V_i \otimes I)^\dagger.\end{aligned} \tag{3.14}$$

For any vector $|\psi\rangle \in \mathcal{H} \otimes \mathcal{H}_2$ now defining $|\psi_i\rangle = (V_i \otimes I)^\dagger |\psi\rangle$, we find that for A' positively definite, we get

$$\langle\psi| (\mathcal{L} \otimes I) A' |\psi\rangle = \sum_i \langle\psi| (V_i \otimes I) A' (V_i \otimes I)^\dagger |\psi\rangle = \sum_i \langle\psi_i| A' |\psi_i\rangle \geq 0, \tag{3.15}$$

thus demonstrating that $\mathcal{L} \otimes I$ takes positive definite operators to positive definite operators.

Let us now take the implication the other way, and derive that any map satisfying these conditions can be written in Kraus form. Here this will only be done under the assumption that $\mathcal{H}$ is finite dimensional. Assume that $\mathcal{L}$ is a map satisfying the conditions above. Let $\mathcal{H}'$ be an identical copy of $\mathcal{H}$, and let $|i\rangle$ and $|i'\rangle$ be orthonormal bases for $\mathcal{H}$ and $\mathcal{H}'$ respectively. Further, define the vector

$$|\phi\rangle = \sum_i |i\rangle \otimes |i'\rangle, \tag{3.16}$$

and the operator

$$\sigma = (\mathcal{L} \otimes I) |\phi\rangle \langle\phi| , \tag{3.17}$$

Since $|\phi\rangle \langle\phi|$ is positive definite, condition c gives that so must σ be. σ is also Hermitian, since any positive operator must be Hermitian. To see this, we note that any operator O can be written as the sum of a Hermitian operator H and an anti-Hermitian operator A, so that

$$\langle\psi| O |\psi\rangle = \langle\psi| H |\psi\rangle + \langle\psi| A |\psi\rangle . \tag{3.18}$$

Since H has only real eigenvalues and A has only imaginary, $\langle\psi| H |\psi\rangle$ must be real and $\langle\psi| A |\psi\rangle$ imaginary. If O is positive, then $\langle\psi| O |\psi\rangle$ is positive and thus real. This means that $\langle\psi| A |\psi\rangle = 0$ for all $|\psi\rangle$, so that in particular all the eigenvalues of A are zero. Thus, clearly $A = 0$ and $O = H$ is Hermitian.

Knowing then that σ is Hermitian, it must have a spectral decomposition

$$\sigma = \sum_k \sigma_k |k\rangle \langle k| , \tag{3.19}$$

with $|k\rangle$ being an orthonormal basis of eigenvectors. The positivity also means that that all the $\sigma_k \geq 0$. This means that 3.19 can in fact be written

$$\sigma = \sum_k |\phi_k\rangle \langle\phi_k| , \tag{3.20}$$

where we have defined $|\phi_k\rangle = \sqrt{\sigma_k} |k\rangle$.

Next, we introduce the conjugate linear map $W : \mathcal{H} \to \mathcal{H}'$, defined by

$$W(\sum_i c_i |i\rangle) = \sum_i c_i^\star \left|i'\right\rangle , \tag{3.21}$$

which we see will have the property that

$$\left\langle i'\right| W(|\psi\rangle) = c_i^\star = \langle\psi|i\rangle. \tag{3.22}$$

Finally we define our Kraus operators V_k by

$$V_k |\psi\rangle = (W(|\psi\rangle))^\dagger |\phi_k\rangle . \tag{3.23}$$

Using these, we find

$$\begin{aligned}
\sum_k V_k |\psi\rangle \langle\psi| V_k^\dagger =& \sum_k W(|\psi\rangle)^\dagger |\phi_k\rangle \langle\phi_k| W(|\psi\rangle) = W(|\psi\rangle)^\dagger \sigma W(|\psi\rangle) \qquad (3.24)\\
=& W(|\psi\rangle)^\dagger (\mathcal{L} \otimes I) |\phi\rangle \langle\phi| W(|\psi\rangle) = \sum_{ij} W(|\psi\rangle)^\dagger (\mathcal{L} \otimes I) |i\rangle \otimes \left|i'\right\rangle \langle j| \otimes \left\langle j'\right| W(|\psi\rangle)\\
=& \sum_{ij} (\mathcal{L} |i\rangle \langle j|) W(|\psi\rangle)^\dagger \left|i'\right\rangle \left\langle j'\right| W(|\psi\rangle) = \sum_{ij} (\mathcal{L} |i\rangle \langle j|) \langle i|\psi\rangle \langle\psi|j\rangle\\
=& \mathcal{L} \sum_{ij} \langle i|\psi\rangle \langle\psi|j\rangle |i\rangle \langle j| = \mathcal{L}(|\psi\rangle \langle\psi|),
\end{aligned}$$

thus demonstrating the Kraus form for pure states. Since any state can be written as a linear combination of pure states, linearity of $\mathcal{L}$ implies that theorem 1 holds for all states. □

3.3 Discussion of the conditions for Kraus Decomposition

Using theorem 1 we could have derived 3.9 in a much simpler fashion: It is easily seen that the map taking $\rho(0) \to \rho(t)$ in 3.2 satisfies all the conditions of the theorem, so that 3.9 follows directly. In fact theorem 1 can be used to argue for a time development on this form in a much wider setting than that of factorizing initial conditions: we will have such time development as long as it satisfies the conditions a - c, no matter the initial conditions. To write things out explicitly, the development of an open system will have the form 3.9 if and only if

(a) The state at times t can be expressed as a function of the initial state: $\rho_S(t) = \mathcal{G}_t(\rho_S(0))$.

(b) The functions $\mathcal{G}_t$ are linear: $\mathcal{G}_t(A) = \mathcal{G}_t A$.

(c) $\mathcal{G}_t$ are trace preserving.

(d) $\mathcal{G}_t$ are completely positive.

Of these conditions we note that already the first one is discussable: The reduced state of S will not only depend on the initial state of S, but on the state of the full system T. In order to claim that it is a function of the reduced state alone we must regard the remaining information as fixed in some way. When the initial state is in factorized form, as in 3.2 this can be done by simply regarding $\rho_E(0)$ as fixed. In the more general case however, it is difficult to see precisely what it is we should regard as fixed. Due to the ambiguity of this condition and the linearity condition which is strongly connected to it, I will delay the discussion of these until after I have dealt with the two remaining ones, which are much simpler.

First, there is not even much to say about c. It must obviously be satisfied since any valid state must develop into another valid state operator with trace 1, and linearity (if we accept this) gives that all other traces must then also be preserved. Condition d must also always be satisfied: First, we note that this would have been easy to see if the condition had involved just plain positivity instead of the more complicated 'complete positivity'. Then this would have followed simply from the fact that any state operator, which is positive, must develop into another positive state operator. Also, any non zero positive operator with a trace can be rescaled to form a density operator.

Concerning this, one might ask why it is at all necessary to demand complete positivity instead of just plain positivity. I at least, would say it seems intuitive that the later should imply the former (the definition of complete positivity is explained in condition c of Kraus' theorem). The answer is that in this case as in many others intuition is simply wrong. It does in fact not: A simple example of a map which satisfies conditions a - c as well as positivity, but which is never the less not completely positive is to take the transpose of an operator with respect to some basis:

$$\mathcal{L}_{\mathcal{T}}(A) = \sum_{ij} |i\rangle \langle j| A |i\rangle \langle j| \tag{3.25}$$

This map is obviously linear, and it is easy to verify that it is trace preserving. Positivity also follows easily from the definition: $\langle\psi| \mathcal{L}_{\mathcal{T}}(A) |\psi\rangle$ becomes $\langle\phi| A |\phi\rangle$, where $|\phi\rangle = \sum_i \langle\psi|i\rangle |i\rangle$. Complete positivity however is not satisfied, as will now be demonstrated. The example is taken from [10].

Consider a simple two level system, and define $\mathcal{L}_{\mathcal{T}}$ as the transpose with respect to the basis $\{|1\rangle, |2\rangle\}$ of this space. We let also the second Hilbert space $\mathcal{H}_2$ from condition c in theorem 1 describe such a two level system, and we look at the effect of the map $\mathcal{L}_{\mathcal{T}} \otimes I$ on the state operator corresponding to the maximally entangled state $\frac{1}{\sqrt{2}}(|1\rangle \otimes |2\rangle + |2\rangle \otimes |1\rangle)$. This operator will be

$$\rho = \frac{1}{2}(|1\rangle \langle 1| \otimes |2\rangle \langle 2| + |1\rangle \langle 2| \otimes |2\rangle \langle 1| + |2\rangle \langle 1| \otimes |1\rangle \langle 2| + |2\rangle \langle 2| \otimes |1\rangle \langle 1|), \tag{3.26}$$

which means we will have

$$\begin{aligned}(\mathcal{L}_\mathcal{T}\otimes I)\rho = &\frac{1}{2}(\mathcal{L}_\mathcal{T}(|1\rangle\langle 1|)\otimes|2\rangle\langle 2| + \mathcal{L}_\mathcal{T}(|1\rangle\langle 2|)\otimes|2\rangle\langle 1| \\ &+ \mathcal{L}_\mathcal{T}(|2\rangle\langle 1|)\otimes|1\rangle\langle 2| + \mathcal{L}_\mathcal{T}(|2\rangle\langle 2|)\otimes|1\rangle\langle 1|) \\ = &\frac{1}{2}(|1\rangle\langle 1|\otimes|2\rangle\langle 2| + |2\rangle\langle 1|\otimes|2\rangle\langle 1| + |1\rangle\langle 2|\otimes|1\rangle\langle 2| + |2\rangle\langle 2|\otimes|1\rangle\langle 1|).\end{aligned} \tag{3.27}$$

We now define the vector $|\psi\rangle = |1\rangle\otimes|1\rangle - |2\rangle\otimes|2\rangle$, and it is easily seen that

$$\langle\psi|\,(\mathcal{L}_\mathcal{T}\otimes I)\rho\,|\psi\rangle = -1, \tag{3.28}$$

which means $(\mathcal{L}_\mathcal{T}\otimes I)(\rho)$ is not positively definite even though ρ, as a valid state operator is. This again means $\mathcal{L}_\mathcal{T}\otimes I$ is not a positive map, and finally that $\mathcal{L}_\mathcal{T}$ is not completely positive.

Knowing then that complete positivity is not equivalent to positivity, we will need to explain in some other way why condition d must be satisfied. To do this, we expand our total system T by a third system S_2 which is not coupled to it, and discuss the development of $S\cup S_2$. If the development of S is described by $\mathcal{G}_t$, the development of $S\cup S_2$ will be given by the super operator $\mathcal{G}_t\otimes I$, since S_2 is not affected by the time development. We assume here not only that S_2 does not interact with S, but also that it has no self-contributions to the Hamiltonian. Now, the map $\mathcal{G}_t\otimes I$ takes the initial state of $S\cup S_2$ to the state at time t, and thus it sends valid state operators to valid state operators. As was explained above this means that $\mathcal{G}_t\otimes I$ must be positive. Since the system S_2 can be described by a Hilbert space of any dimension, the condition follows.

By the preceding discussion, we see that if a and b are assumed, the conditions c and d must be satisfied by any valid development of a state operator. Having now dealt with this, we may turn back to the conditions a and b themselves. As already mentioned, to assume condition a is the same as to in some way regard the information of ρ_T that is not contained in ρ_S as being fixed. This statement is obviously very imprecise, and it can obviously be interpreted in a large number of ways. It is not hard to realize that whether the functions $\mathcal{G}_t$ are linear will depend on precisely what way we regard this information as being fixed. With other words, the questions of whether the conditions a and b are justified are strongly connected.

Before we go into this however, we should say something about why we would at all expect $\mathcal{G}_t$ to be linear. Well, fist of all we know that closed systems develop linearly. Assuming that open systems also do this would then be the simplest generalization. Secondly, it is possible to prove this as long as one limits one self to what is called convex linearity. This means that in the linearity condition $\mathcal{G}_t(aA+bB) = a\mathcal{G}_tA+b\mathcal{G}_tB$ we demand the coefficients a and b to be positive and sum to 1. These coefficients can then be interpreted as probabilities, while the state operator $C = aA + bB$ can be interpreted as representing a situation where the system S is prepared in the state A with probability a and in the state B with probability b. At time t it will then be in the state $\mathcal{G}_tA$ with probability a and $\mathcal{G}_tB$ with probability b. The actual state operator will then be $a\mathcal{G}_tA + b\mathcal{G}_tB$, which proves convex linearity. However, to demand this type of probabilistic interpretation of the state operators actually means we are limiting the possible ways in which the external information can be fixed.

In [2] and [10] it is in fact claimed that convex linearity is all that is needed for Kraus decomposition. Upon examining their proof one will however discover that this actually requires full linearity. More precisely this is in the equivalent of equation 3.24, where linearity beyond just convex is clearly employed. Because of this I have chosen to write down full linearity as the condition for Kraus decomposition, as is also done in [11]. The condition is thus in need of further justification.

One possible way of regarding the external information as fixed, which is used at one place in [2], is to introduce a *reference state* b of the environment E. For instance b could simply be $\rho_E(0) = \mathrm{Tr}_S\rho_T(0)$. What one then chooses to regard as fixed, is the operator $\mathcal{Q}\rho_T(0) = \rho_T(0) - \rho_S(0)\otimes b$. The notation here will be explained in a later chapter. In this one the important point is just that when $\mathcal{Q}\rho_T(0)$ is fixed,

$\rho_S(t)$ can be expressed as a function of $\rho_S(0)$ through the relation

$$\rho_S(t) = \mathcal{G}_t(\rho_S(0)) = \mathrm{Tr}_E(U(t)(\rho_S(0) \otimes b)U^\dagger(t)) + \mathrm{Tr}_E(U(t)(\mathcal{Q}\rho_T(0))U^\dagger(t)). \tag{3.29}$$

We note however that the map $\mathcal{G}_t$ is in this case not linear, since it contains the inhomogeneous term $\mathrm{Tr}_E(U(t)(\mathcal{Q}\rho_T(0))U^\dagger(t))$. Thus $\mathcal{G}_t$ obviously does not satisfy the conditions for Kraus decomposition. In fact 3.29 violates also convex linearity, so that the probability interpretation can not be used.

If we wish the probability interpretation to apply, and in particular if we want $\mathcal{G}_t$ to satisfy the conditions for Kraus decomposition, we must clearly find some other way of regarding the Environmental information as fixed. Let us examine precisely what it is we need: We want to express $\rho_S(t)$ as a function of $\rho_S(0)$, whereas in reality it is a function of $\rho_T(0)$. Clearly the way to solve this is to assume that $\rho_T(0)$ is itself a function of $\rho_S(0)$: that is $\rho_T(0) = \mathcal{L}(\rho_S(0))$. This is in fact precisely what was done in 3.29, with the function $\mathcal{L}$ being simply $\mathcal{L}(\rho) = \rho \otimes b + \mathcal{Q}\rho_T(0)$.

However, with this choice for $\mathcal{L}$, $\mathcal{G}_t$ did not satisfy the conditions for Kraus decomposition. It is not hard to see that if we want to satisfy these conditions, the map $\mathcal{L}$ must also satisfy the same three conditions of linearity, trace preservation and complete positivity. In addition to this it must clearly also satisfy the condition that $\mathrm{Tr}_E\mathcal{L}A = A$, since this must be the case if it takes $\rho_S(0)$ to $\rho_T(0)$. The case of factorizing initial conditions gives the simplest example of a map $\mathcal{L}$ that satisfies all of these conditions: In this case is is simply given by $\mathcal{L}A = A \otimes \rho_E(0)$. Other examples are difficult to construct explicitly, but the mentioned constraints of the map $\mathcal{L}$ are certainly not so limiting as to exclude their existence.

Having now gone through each of the conditions for Kraus decomposition in some detail, we are ready to make some conclusion as to whether they are justified. The answer seems to be that this depends entirely on the way in which the external information is fixed: As long as one can do this in the right way, one can make sure that the Kraus conditions are satisfied. And if this is not done in the right way it is easy to construct examples where they are not. However, since the way we fix this external information is to a large degree up to ourselves, it is perhaps not so unreasonable to assume that we can always do this in such a way that the Kraus conditions hold. If this is indeed the case, then it is well justified to take 3.9 to be the correct generalization of unitary time development for open systems. In this thesis, we shall in any situation where we have a concrete model for T assume factorizing initial conditions, in which case 3.9 is in any case certain to hold.

Chapter 4

Markovian descriptions of open systems

4.1 Markovianness and Quantum Dynamical Semigroups

In the previous chapter we came to the conclusion that the best generalization of the unitary time development postulate $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$ or alternatively $\rho(t) = U(t)\rho(0)U(t)^\dagger$, is the Kraus decomposition 3.9. In the case of closed systems, unitary time development can be used to derive the existence of differential equations describing the development of the state. In the pure state formulation this is the Schrödinger equation, $\hbar i|\dot{\psi}\rangle = H\,|\psi\rangle$, while in the density operator formulation it is the quantum Liouville equation, $\hbar i\dot{\rho} = [H, \rho]$. The Hamiltonian operator H is defined from the time development operator $U(t)$ by $H(t) = \hbar i\dot{U}(t)U(t)^\dagger$.

With this in mind, it becomes a natural question to ask whether the Kraus decomposition 3.9 can be used to argue for the existence of a differential equation describing the development of states also in open systems. The answer turns out to be no. 3.9 is not enough to assure the existence of such an equation, and indeed not all open systems can be described by a differential equation. The reason for this is that for a system to be described by a differential equation, it must be manifestly *Markovian*. This means that it must be possible to determine the state at time t from the state at any earlier time t'.

3.9 merely says it is possible to determine the state at time t from the state at time 0, and thus it is not necessarily Markovian. Of course, on a superficial level this seem to be the case also for closed systems, since the time development postulate $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$ expresses $|\psi(t)\rangle$ in terms of $|\psi(0)\rangle$. It is however easy to see that closed systems are in fact Markovian. This is due to the fact that unitary operators are always invertible, so that one can actually express $|\psi(t)\rangle$ in terms of the state at any time t' through the simple relation $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle = U(t)U_{t'}^\dagger\,|\psi(t')\rangle$.

The time development operator $\mathcal{G}_t$ defined by 3.9 is however not necessarily invertible. Thus, if we wish to make use of Markovianness we will have to make this an assumption. This chapter deals with the description of open systems where this assumption is made. I should stress however that this is not always justified: When a system is coupled to an environment, as is the case with open systems, it is reasonable to believe that the environment will be able to act as a memory, since it is capable of storing information about the system. It would then seem that the systems behavior could be influenced by its past states through this external memory, and not only by its present state. As we will see it turns out even so that open systems often has an exact Markovian description. This is however not always the case, so if one wishes a completely general description this can not be Markovian. A particular non-Markovian description will be dealt with in the next chapter.

In addition to Markovianness we will also assume linearity. This is already assumed in the Kraus form, and so in generalizing this to a Markovian expression we might as well keep this assumption. In total then, we assume that for any pair of times $0 \leq t' \leq t$ we can express the state $\rho(t)$ as

$$\rho(t) = \mathcal{G}_{t'\to t}\rho(t'). \tag{4.1}$$

The set of super operators $\mathcal{G}_{t'\to t}$ obviously satisfies

$$\mathcal{G}_{t'\to t''}\mathcal{G}_{t\to t'} = \mathcal{G}_{t\to t''} \tag{4.2}$$

for any $t \leq t' \leq t''$. If they in addition to this are trace preserving and completely positive they are referred to as a *quantum dynamical Semigroup*[1][2]. This name makes reference to the concept of an algebraic semigroup, which is a mathematical structure that has all the same properties of a group, except that all elements does not necessarily have an inverse. This is of course because 4.2 is a sort of group property, while at the same time there is no guaranty that the operators are invertible.

One should note that one does loose generality by assuming that a Markovian development is a quantum dynamical semigroup. Obviously $\mathcal{G}_{t'\to t}$ will have to be trace preserving, but they need not be completely positive nor even positive. The reader might find this somewhat puzzling, since this condition was easily shown to be true in the case of the original Kraus form 3.9. Should this argument not be generalizable to the Markovian case? Well, in fact no. An important point in the original demonstration was that $\mathcal{G}_t$ acts on the states at $t = 0$, at which the system can be in any state. All of these must then be sent to positive operators. However, at later times t' only states that are in the image of $\mathcal{G}_{t'}$ are possible, and thus we have no guarantee that states outside of this image will develop into positive operators.

Thus the operators $\mathcal{G}_{t'\to t}$ need not necessarily be positive, and in the cases where the open system has an exact Markovian description they are in fact often not. Quite often however Markovian descriptions are based on an approximation where one assumes that the memory of the environment is 'short'. This short memory could also be used to argue that the environment in a way 'does not know what time it is', so that the maps $\mathcal{G}_{t'\to t}$ can only depend on time differences. That is, we would have $\mathcal{G}_{t'\to t} = \mathcal{G}_{t-t'}$. In this case they would have to be completely positive since the operators $\mathcal{G}_t$ are. If this is the case they will form a quantum dynamical semigroup, and in particular they satisfy the conditions for Kraus decomposition so that 4.1 becomes

$$\rho(t) = \sum_i V_i(t,t')\rho(t')V_i(t,t')^\dagger, \text{ with} \tag{4.3}$$

$$\sum_i V_i(t,t')^\dagger V_i(t,t') = I. \tag{4.4}$$

In section 4.3 I will show that equation 4.3 can be used to derive a generalization of the Schrödinger/Liouville equation.

For now however let us return to general Markovian operators $\mathcal{G}_{t'\to t}$ that does not necessarily form a dynamical semigroup. As long as these operators are differentiable, 4.1 can always be used to derive a differential equation for $\rho_S(t)$: We define the *Markovian generator* $\mathcal{M}_t$ in the following way:

$$\mathcal{M}_t = \frac{\mathrm{d}}{\mathrm{d}t'}\mathcal{G}_{t\to t'}\big|_{t'=t}. \tag{4.5}$$

From this and 4.1 we see that $\rho_S(t)$ will in fact satisfy the equation

$$\dot{\rho}_S = \mathcal{M}_t\rho_S. \tag{4.6}$$

Of course this expression in a way already forms a generalization of the Liouville equation. But this expression is really to general to be used for practical modeling: We have no idea how to choose the generator $\mathcal{M}_t$ so as to make sure the states develop in a meaningful way where they remain positively definite. When we start out with a quantum dynamical semigroup however, the generator can be put into a standard form that always has this property. Just like the Liouville equation and the Kraus decomposition 3.9 this standard form also has the advantage that it is expressed in terms of operators acting on the Hilbert space $\mathcal{H}_S$.

4.2 Markovianness and invertibility.

I mentioned above that the reason unitary time development is by necessity Markovian is that unitary operators are always invertible, and similarly that open systems are not necessarily Markovian since the time development operators $\dot{\mathcal{G}}_t$ are not necessarily invertible. However, if they happen to be invertible

then the development will be Markovian. This can be shown in precisely the same way as in the unitary case: Assume that for $t > 0$ our open system S has the development $\rho_S(t) = \mathcal{G}_t\rho(0)$. Assume further that in the range $0 \leq t \leq T$ these operators are invertible. In this range, $\rho_S(t)$ can be expressed as $\rho_S(t) = \mathcal{G}_t\mathcal{G}_{t'}^{-1}\rho_S(t')$. If we now simply define $\mathcal{G}_t\mathcal{G}_{t'}^{-1} = \mathcal{G}_{t'\to t}$, we see that this becomes 4.1, our definition of Markovianness. This means that as long as the operators $\mathcal{G}_t$ are in fact invertible, the system has (in principle) an exact Markovian description.

Concerning this, two points should be noted: First, even if the original operators $\mathcal{G}_t$ satisfies the conditions for Kraus decomposition, the operators $\mathcal{G}_t\mathcal{G}_{t'}^{-1} = \mathcal{G}_{t'\to t}$ need in general not. The reason for this was explained above. Secondly, we should note that it is no at all unreasonable to assume the operators $\mathcal{G}_t$ to be invertible in some interval $0 \leq t \leq T$. As long as we assume the system S to have finite dimension N this is in fact even provable:

In this case the operators $\mathcal{G}_t$ will have well defined determinants. Since the determinants are continuous functions of the operators and the operators are assumed to vary continuously with time, the determinant $\mathrm{Det}\,\mathcal{G}_t$ must also vary continuously with time. Since $\mathrm{Det}\,\mathcal{G}_0 = \mathrm{Det}\,\mathcal{I} = 1$ ($\mathcal{I}$ being the identity super operator) and we must have $\mathrm{Det}\,\mathcal{G}_t = 0$ in order for $\mathcal{G}_t$ not to be invertible, it follows that $\mathcal{G}_t$ must be invertible in some interval after 0.

I do not know if this proof can be generalized to infinite dimensional systems, and under full generality I would in fact expect that it can not. However, I would also expect that the result only fails under very special circumstances. So I would say it is always well justified to assume invertibility, and thus Markovianness in some interval $0 \leq t \leq T$. As of yet this does of course not have any practical applications, since we know of no way to find this description. In particular we have no way to find the generator $\mathcal{M}_t$. In the next chapter we will however see that this generator can actually be approximated in a systematic fashion.

Having now demonstrated that invertible time development implies Markovianness, we might wonder whether these two properties are even equivalent. That is, we might wonder whether Markovianness also implies invertibility. In general this is of course not the case: There is no way to argue from 4.1 alone that the operators $\mathcal{G}_{t'\to t}$ must be invertible. However, if we also assume differentiability, so that the development is described by 4.6, then invertibility becomes at least very plausible.

To see this, we note that 4.6 implies that the operators $\mathcal{G}_{t'\to t}$ will themselves satisfy the equation

$$\dot{\mathcal{G}}_{t'\to t} = \mathcal{M}_t\mathcal{G}_{t'\to t}, \tag{4.7}$$

with the initial conditions $\mathcal{G}_{t'\to t'} = I$. Under the assumption of existence and uniqueness of solutions (and of course any self respecting physicist would take a suggestion to the contrary as a personal insult), this *initial value problem* can be used to *define* $\mathcal{G}_{t'\to t}$ also for $t < t'$. It then seems very intuitive that the operator $\mathcal{G}_{t\to t'}$ should be the inverse of $\mathcal{G}_{t'\to t}$, and in fact this can be demonstrated to be the case:

First, take note that if the solution to 4.7 is unique under the initial condition $\mathcal{G}_{t'\to t'} = I$, then it must also be unique under any other initial condition. This follows simply from linearity, since one can just add together solutions to obtain new initial values. Next, consider the product of operators $\mathcal{G}_{t'\to t''}\mathcal{G}_{t''\to t}$. This product clearly satisfies the equation $\frac{\mathrm{d}}{\mathrm{d}t''}\mathcal{G}_{t'\to t''}\mathcal{G}_{t\to t'} = \mathcal{M}_{t''}\mathcal{G}_{t'\to t''}\mathcal{G}_{t\to t'}$, as well as the initial condition $\mathcal{G}_{t'\to t'}\mathcal{G}_{t\to t'} = \mathcal{G}_{t\to t'}$. The uniqueness of solutions to this initial value problem them implies that the product must equal the operator $\mathcal{G}_{t\to t''}$. Now simply setting $t'' = t$, we see that $\mathcal{G}_{t\to t'}$ is indeed the inverse of $\mathcal{G}_{t'\to t}$.

Of course this argument hinges greatly on the assumption of existence and uniqueness of solutions to 4.7. This can however be safely assumed as long as the generators $\mathcal{M}_t$ satisfies *appropriate* conditions of continuity. To summarize then, we see that Markovianness and invertibility can be thought of as equivalent,but only if we make additional assumptions of differentiability and continuity of the operators $\mathcal{M}_t$.

4.3 The Lindblad equation

I mentioned in the preceding that we can derive a generalization of the Liouville equation if we assume that the system S is described by a quantum dynamical semigroup. This equation is known as the *Lindblad equation*. A quantum dynamical semigroup can be expressed using the Lindblad Equation as long as the super operators $\mathcal{G}_{t'\to t}$ are bounded. This was in fact proven by Lindblad[8], which is why the equation was named after him. I will now state this theorem, but the proof will only be given for finite dimensional Hilbert spaces.

Theorem 2. Lindblad Equation.

Assume that some state operator $\rho(t)$ acting on a Hilbert space $\mathcal{H}$ has a time development that can be expressed as 4.3. Assume further that the operators V_i in this expression are bounded and differentiable. Then $\rho(t)$ satisfies the *Lindblad Equation*, which can be expressed using either of the two following standard forms:

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] + \sum_{ij} a_{ij}(F_i\rho F_j^\dagger - \frac{1}{2}\{F_j^\dagger F_i, \rho\}), \tag{4.8}$$

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] + \sum_{i} \gamma_i(A_i\rho A_i^\dagger - \frac{1}{2}\{A_i^\dagger A_i, \rho\}), \tag{4.9}$$

where H is a Hermitian operator, $\gamma_i > 0$ and $\mathrm{Tr}F_i^\dagger F_j = \mathrm{Tr}A_i^\dagger A_j = \delta_{ij}$. Also, H, a_{ij}, γ_i and A_i may in general depend on time, while the operators F_i does not.

Proof. The proof will only be given in the case where $\mathcal{H}$ has finite dimension. It is a slightly modified version of one that is fond in [2]. Let us denote the dimension N. The space $L(\mathcal{H})$ of linear operators on $\mathcal{H}$ then forms a N^2 dimensional space. We define an inner product on this space as $\mathrm{Tr}A^\dagger A$, and we pick a basis for $L(\mathcal{H})$ which is orthonormal with respect to this inner product. We specifically pick one of the basis vectors to be $\frac{1}{\sqrt{N}}I$, and we denote the remaining N^2-1 operators as F_i. Note that these operators being ortogonal to $\frac{1}{\sqrt{N}}I$ means that they are traceless. The V_i operators from 4.3 can then be expanded as

$$V_j = \frac{1}{N}\left(\mathrm{Tr}V_j\right)\cdot I + \sum_i \left(\mathrm{Tr}F_i^\dagger V_j\right)\cdot F_i, \tag{4.10}$$

which means we can rewrite this equation as

$$\begin{aligned}\rho(t) =& \frac{1}{N^2}\sum_i |\mathrm{Tr}V_i|^2\cdot\rho(t') + \frac{1}{N}\sum_{ij}(\mathrm{Tr}V_i\mathrm{Tr}V_i^\dagger F_j\cdot\rho(t')F_j^\dagger + \mathrm{Tr}V_i^\dagger\mathrm{Tr}F_j^\dagger V_i\cdot F_j\rho(t')) \\ &+ \sum_{ijk}\mathrm{Tr}F_j^\dagger V_i\mathrm{Tr}V_i^\dagger F_k\cdot F_j\rho(t')F_k^\dagger \\ =& f\rho(t') + F\rho(t') + \rho(t')F^\dagger + \sum_{jk} c_{jk}F_j\rho(t')F_k^\dagger,\end{aligned} \tag{4.11}$$

where we have now defined

$$f = \frac{1}{N^2}\sum_i |\mathrm{Tr}V_i|^2, \tag{4.12}$$

$$F = \frac{1}{N}\sum_{ij}\mathrm{Tr}V_i^\dagger\mathrm{Tr}F_j^\dagger V_i\cdot F_j, \tag{4.13}$$

$$c_{jk} = \sum_i \mathrm{Tr}F_j^\dagger V_i\mathrm{Tr}V_i^\dagger F_k. \tag{4.14}$$

We then take the derivative of 4.11 with respect to t at $t = t'$ to get

$$\dot{\rho} = \dot{f}\rho + \dot{F}\rho(t') + \rho(t')\dot{F}^\dagger + \sum_{ij} \dot{c}_{ij} F_i \rho F_j^\dagger = -\frac{i}{\hbar}[H, \rho] + \{G, \rho\} + \sum_{ij} a_{ij} F_i \rho F_j^\dagger, \tag{4.15}$$

with further definitions of the Hermitian operators H and G, and the coefficients a_{ij}:

$$H = \frac{\hbar}{2i}(\dot{F}^\dagger - \dot{F}), \tag{4.16}$$

$$G = \frac{1}{2}(\dot{f}I + \dot{F}^\dagger + \dot{F}), \tag{4.17}$$

$$a_{ij} = \dot{c}_{ij}. \tag{4.18}$$

The maps 4.3 preserves traces, so we must have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\rho = 2\mathrm{Tr}G\rho + \sum_{ij} a_{ij}\mathrm{Tr}F_i\rho F_j^\dagger = \mathrm{Tr}(2G + \sum_{ij} a_{ij}F_j^\dagger F_i)\rho = 0. \tag{4.19}$$

Since this means that the operator $2G + \sum_{ij} a_{ij}F_j^\dagger F_i$ is orthogonal to all operators it must be identically 0, so that $G = -\frac{1}{2}\sum_{ij} a_{ij}F_j^\dagger F_i$. This finally gives us the Lindblad equation in its first standard form 4.8.

Next, we want to demonstrate that the $N^2 - 1 \times N^2 - 1$ matrix a of the coefficients a_{ij} is Hermitian and positive definite. We first show this for the corresponding matrix c of the coefficients c_{ij}. Hermiticity follows straight forward from the definition 4.14, and to prove positivity we calculate

$$\begin{aligned} v^\dagger c v &= \sum_{jk} v_j^\star c_{jk} v_k = \sum_{jk} v_j^\star \sum_i \mathrm{Tr}F_j^\dagger V_i \cdot \mathrm{Tr}V_i^\dagger F_k v_k \\ &= \sum_i \mathrm{Tr}\sum_j v_j^\star F_j^\dagger V_i \cdot \mathrm{Tr}\sum_k V_i^\dagger F_k v_k = \sum_i |\mathrm{Tr}\sum_j v_j^\star F_j^\dagger V_i|^2 \geq 0, \end{aligned} \tag{4.20}$$

for any vector v. Hermiticity of a now also follows straight forward from 4.18 and the Hermiticity of c. To show positivity we first calculate

$$\begin{aligned} c_{jk}(t,t) &= \sum_i \mathrm{Tr}F_j^\dagger V_i \mathrm{Tr}V_i^\dagger F_k = \sum_{lm} \langle l| F_j^\dagger \left(\sum_i V_i |l\rangle \langle m| V_i^\dagger\right) F_k |m\rangle \\ &= \sum_{lm} \langle l| F_j^\dagger |l\rangle \langle m| F_k |m\rangle = \mathrm{Tr}F_j^\dagger \mathrm{Tr}F_k = 0, \end{aligned} \tag{4.21}$$

which means we have $v^\dagger c(t,t)v = 0$ for all v. Since $v^\dagger c(t,t')v \geq 0$ for $t' > t$, this further means we must have

$$\frac{\mathrm{d}}{\mathrm{d}t'} v^\dagger c(t,t) v = v^\dagger a(t) v \geq 0. \tag{4.22}$$

The fact that a is Hermitian and positive means we can diagonalize it as $a = u\gamma u^\dagger$, or

$$a_{ij} = \sum_k u_{ik}\gamma_k u_{jk}^\star, \tag{4.23}$$

$$\gamma_k \geq 0. \tag{4.24}$$

Inserting this into 4.8 while defining the operators

$$A_j = \sum_i u_{ij} F_i \tag{4.25}$$

then gives us the Lindblad equation in its second standard form 4.9. □

As mentioned the full proof in [8] expands this result to infinite dimensional systems, but only when the Kraus operators are bounded. Of course one can not generally expect this to be the case, but the fact is that there are no examples of a physically relevant quantum dynamical semigroup where it can not be expressed using the Lindblad equation[2]. This is the case even when the Kraus operators are not bounded. So even though we have no formal proof to support us in all cases: if we wish to study quantum dynamical semigroups we can usually assume the Lindblad equation to be well suited.

Of course, not all open quantum systems can be described using a quantum dynamical semigroup, and in these cases we can neither assume the Lindblad equation to apply. In particular this will be the case if the system does not satisfy the Markovian condition 4.1, or if the super operators $G_{t'\to t}$ are not completely positive.

Finally I should mention that the constituents of 4.9 have simple interpretations that are useful for modeling: We first note that if all the γ_i are set to 0, the equation reduces to the standard Liouville equation with H being the Hamiltonian. It is then reasonable to keep the interpretation that H is a Hamiltonian describing unitary processes also in the general case. Terms involving the operators A_i are what separates 4.9 from the standard unitary equation, and thus these operators must describe non-unitary processes. It then becomes reasonable to interpret the positive coefficients γ_i simply as the rates by which these processes occur. This will later be exemplified.

4.4 The Redfield equation

The Lindblad equation described in the previous section is an example of an attempt to describe open quantum systems using a differential equation. The derivation of this equation was merely based on a set of more or less justified assumptions about the development, which in particular involved the condition that it forms a quantum dynamical semigroup. It did not in any way involve a discussion of the development of the total closed system T. Thus we have as of yet no information about the connection between the Markovian description of the reduced system S and the unitary development of T.

Note that his connection is something we would like to understand, since our present day understanding of elementary interactions are formulated in terms of unitary models. Given a particular quantum system S coupled to a particular type of environment E we might have a good understanding of the interactions between these, and we could thus easily construct a unitary model for the total system T in terms of some Hamiltonian H_T. It would then be nice to have some way to turn this model into a model for S alone, since this would then be a model based on fundamental principles. Sadly, the Lindblad equation 4.9 provides no such way.

Luckily there does exist ways to reduce the model for T into models for S alone. However, in order for such descriptions to both be exact and completely general they must be able to deal also with non-Markovian behavior. This means they can not be formulated in terms of a simple differential equation like 4.9 since these always gives rise to Markovian behavior. The treatment of such methods will therefore be postponed to the next chapter. One can of course reduce the generality of the description to only encompass systems that have invertible time development operators $\mathcal{G}_t$, so that as explained in section 4.2 they can be treated as Markovian. In these cases it turns out one can find a reduced description of S in terms of a differential equation of type 4.6 that is still exact. The derivation of this however, relies heavily on the mentioned Non-Markovian method, and this to will be postponed to the next chapter.

Finally, we might reduce the requirement that the description be exact, and base the derivation only on some heuristically justified approximations. This is what we will do in this section, and the equation to be derived is known as the Redfield equation[2] due to its original derivation by Redfield[12]. The approximations that are used are based on the assumption that the interactions with the environment are weak, or alternatively that the environment is large. I stress again that the justifications I will give for these approximations are meant to be heuristic only. A more rigorous argument can be provided by starting out with the exact Markovian equation I mentioned earlier. This will also be done in the next chapter.

Now, assume that we are given some open system S coupled to an environment E, and that they are

described by the Hamiltonian $H_T = H_S + H_E + H_{SE}$. Assume further that we have factorizing initial conditions as in 3.2. The Redfield equation will be expressed in the interaction picture. In this picture the total system T will satisfy the interaction picture Liouville equation $i\hbar\dot{\rho}_T = [H_{SE}, \rho_T]$. We integrate this equation from 0 to t and insert the result back into the original equation. This gives us

$$\dot{\rho}_T = \frac{1}{i\hbar}[H_{SE}(t), \rho_S(0) \otimes \rho_E(0)] - \frac{1}{\hbar^2}\int_0^t [H_{SE}(t), [H_{SE}(t'), \rho_T(t')]]dt'. \tag{4.26}$$

Now, in addition to the assumption of weak interactions we also assume that $\mathrm{Tr}_E(H_{SE}\rho_E(0)) = 0$. This assumption is also made in the entire next chapter, and it will be justified there (see equation 5.2). With this assumption in mind, we now take the partial trace over E of 4.26 and get

$$\dot{\rho}_S = -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_E[H_{SE}(t), [H_{SE}(t'), \rho_T(t')]]dt'. \tag{4.27}$$

This is clearly an exact differential equation for ρ_S, but it depends explicitly on the state of the full system T. We thus make our first approximation, which is to say that if the environment is large and the interactions with it are weak, then the state of the environment will only be very weakly perturbed from its free evolution. In the interaction picture we may then approximate ρ_T as $\rho_T(t) = \rho_S(t) \otimes \rho_E(0)$, which turns 4.27 into

$$\begin{aligned}\dot{\rho}_S &= -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_E[H_{SE}(t), [H_{SE}(t'), \rho_S(t') \otimes \rho_E(0)]]dt' \qquad (4.28)\\ &= -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_E[H_{SE}(t), [H_{SE}(t-t'), \rho_S(t-t') \otimes \rho_E(0)]]dt'.\end{aligned}$$

Considering $\rho_E(0)$ as fixed, this equation depends only on the state of S, which is already a significant simplification. However, the equation takes the form of an integro-differential equation involving the states $\rho_S(t')$ at earlier times than t. These types of equations are often referred to as memory equations[1], and they are obviously not Markovian.

In the next chapter these types of equations will be discussed in larger detail, but here we will make a second approximation in order to get a Markovian equation: if again the environment is big, then we expect information absorbed from S to diffuse around this in such a way as to be less and less available to affect the future behavior of S. In effect we expect the environment to 'forget' the information of S over some characteristic time. If the interactions are weak, we also expect the state of S to change little over this time. What this means concretely is that we expect the last integral in 4.28 to only get significant contributions from times t' where $\rho_S(t-t') \approx \rho_S(t)$. This suggests that our final approximation should be to replace $\rho_S(t-t')$ with $\rho_S(t)$. This finally gives us the Redfield equation:

$$\dot{\rho}_S = -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_E[H_{SE}(t), [H_{SE}(t-t'), \rho_S(t) \otimes \rho_E(0)]]dt', \tag{4.29}$$

which is Markovian. If the memory loss of the environment is very fast we can make even a further approximation, which is to set the integration limit to infinity:

$$\dot{\rho}_S = -\frac{1}{\hbar^2}\int_0^\infty \mathrm{Tr}_E[H_{SE}(t), [H_{SE}(t-t'), \rho_S(t) \otimes \rho_E(0)]]dt'. \tag{4.30}$$

This equation only depends on t through the operators, so that if the original Hamiltonian H_T in the Schrödinger picture does not depend on time, then unlike 4.29, 4.30 would give rise to time translationally invariant behavior. Since this really simplifies the process of solving the equation, and the justification for 4.30 is really only based on the same approximations as 4.29 in any case, 4.30 is the equation one typically uses in practice.

We now have two different Markovian differential equations describing the development of an open quantum system: The Lindblad equation, which is simply based on the assumption that the open system

forms a quantum dynamical semigroup, and the Redfield equation which is based on approximations of the unitary development of the total system T. It then becomes a natural question whether there is any connection between these equations. In particular we wonder whether the Redfield equation can be written in Lindblad form as 4.9. This is essentially the same as asking whether the Redfield equation describes a quantum dynamical semigroup.

Well, we already know it is Markovian and it is easily shown that it preserves traces, so the real question is whether it is completely positive. As explained 4.30 very well might have a time independent generator (in the Schrödinger picture). As explained in section 4.1 this would mean the development would have to be completely positive in order for state operators to remain state operators. This however does not actually guarantee the condition: 4.30 is based on approximations, and we thus have no reason to expect it to preserve state operators as state operators in any more than an approximate sense.

And indeed, according to [4] one can easily construct examples where the Redfield equation does not result in time development that is completely positive. Thus, the Redfield equation does not in general describe a quantum dynamical semigroup, and in particular it can not generally be written in Lindblad form. However, it also turns out that it can always be written is such a form, provided we make one additional approximation: The Redfield equation it self is based on the assumption that the interaction strength is much weaker than a characteristic energy in the environment E (we will get back to this in the next chapter), but to guarantee that it can be written in Lindblad form we must also assume the interaction strength to be much weaker than a characteristic energy in the system S.

More specifically we assume the interaction strength to be much smaller than the typical spacing of energy levels in S. This allows us to ignore interactions which does not conserve the total energy of S and E, an approximation that is some times referred to as the the rotating wave approximation[2]. In [2] this is used together with the Redfield equation 4.30 to derive an equation on the form 4.9 under otherwise completely general conditions. In both of the two models to be studied in this thesis, the rotating wave approximation will be made already at the level of the Hamiltonian H_T.

Chapter 5

A Non-Markovian description of open systems

5.1 The Nakajima Zwanzig equation

In the previous chapter we saw two examples of approximate Markovian differential equations (so called master equations) for the state operator ρ of an open system: The Lindblad equation 4.9 was based on the assumption that the development must form a quantum dynamical semigroup, while the Redfield equation 4.30 was based on the unitary development of the total system T. I also mentioned that under certain assumptions of invertibility, there exists in principle a Markovian generator that describes the system exactly.

In the general case however, where cases without such invertibility must also be included, the system can not necessarily be described in a Markovian fashion. In particular it can not be described by a differential equation, since these are Markovian by their very nature. Thus, some other type of description must be used. The particular description that will be employed in this chapter, is the use of an integro-differential equation: a so called memory equation. Typically this would be an equation on the form

$$\dot{x}(t) = \int_{t_0}^{t} f(t, s, x(s))ds, \tag{5.1}$$

where the function $f(t, s, x)$ is known as the memory kernel. In fact, I briefly mentioned such equations earlier: Equation 4.28, which was just a step in a heuristic argument of the Redfield equation, is clearly an example of such an equation. This equation is however based on precisely the same approximations as 4.30 itself: It assumes the environment to be unperturbed by the interaction with S, and it is therefore only valid in the weak interaction limit. It can thus never really be expected to form a much better description than the Markovian Redfield equations 4.30 or 4.29.

It turns out however that there exists an equation of type 5.1 that describes open systems in an exact manor. To be more precise, given some unitary model of the total system $T = S \cup E$, the state operator $\rho(t)$ that solves this equation is the one found from 3.1. This equation is known as the *Nakajima Zwanzieg equation*[2][9][16]. Its most general formulation can in fact even be applied to systems with completely general initial conditions. In this case however, the equation has inhomogeneous terms and is thus not linear. This means the solution can not be written in Kraus form, and in addition it of course complicates the solution.

Because of this we will in this thesis specialize the equation to factorizing initial conditions, in which case the function $f(t, s, x)$ and thus the entire equation will be linear. For the general discussion see [2]. In addition to factorizing initial conditions we will also assume that

$$\mathrm{Tr}_E\left(H_{SE}\rho_E(0)\right) = \sum_i P_i \left\langle i\right| H_{SE} \left|i\right\rangle = 0, \tag{5.2}$$

where the basis $|i\rangle$ diagonalizes $\rho_E(0)$, P_i are the corresponding eigenvalues and H_{SE} is the interaction part of the Hamiltonian $H_T = H_S + H_E + H_{SE}$ of T. That is, the part of the Hamiltonian that describes interactions between S and E. Note, that 5.2 is also the same as saying that $\mathrm{Tr}_E(\rho_E(0)H_{SE}) = 0$. This condition was also used in section 4.4. The justification was however delayed to this chapter, and this is what I will now attempt:

It seems of course like a weird condition to impose, but it is actually very plausible. The reason for this can be summarized in three points. First, the state $\rho_E(0)$ is often a thermal state, while the interaction operator H_{SE} is often a sum of terms on the form $A_S \otimes B_E$ where $\langle B_E \rangle = 0$ in thermal states. For instance, in quite a lot of models B_E is simply a creation or annihilation operator of some harmonic oscillator. Secondly even if it is not exactly the case, it can be a good approximation. When the interactions between S and E are weak, the expectation value of H_{SE} can be assumed to be essentially zero compared to other relevant quantities.

The third and most important point however, is that as long as the initial state $\rho_E(0)$ of the environment is given, one can always force this condition to be true by doing some shuffling of the terms in the Hamiltonian H_T. In fact, all one needs to to is to add the term $\mathrm{Tr}_E(H_{SE}\rho_E(0))$ to the system Hamiltonian H_S, while subtracting it from H_{SE}. This leaves the dynamics of the total system invariant, while it also assures the fulfillment of condition 5.2. Note that doing this and then simply ignoring the interactions would correspond to a semiclassical approximation.

Now that I have stated the conditions under which the equation will be derived, we may turn to defining a few symbols that will be useful during this derivation. First, we define the super operator $\mathcal{P}$ acting on the state operator space of the total system $T = S \cup E$ as

$$\mathcal{P}\rho_T = \left(\mathrm{Tr}_E\, \rho_T\right) \otimes \rho_E(0), \tag{5.3}$$

with $\rho_E(0)$ being the initial state of the environment. That is, the total system starts out in the factorized form $\rho_T(0) = \rho_S(0) \otimes \rho_E(0)$. In addition to $\mathcal{P}$, we also define the super operator $\mathcal{Q} = \mathcal{I} - \mathcal{P}$ (where $\mathcal{I}$ is again the identity super operator), and to shorten the notation also the super operator $\mathcal{L}$ given by $\mathcal{L}\rho_T = -\frac{i}{\hbar}[H_{SE}, \rho_T]$. We shall refer to $\mathcal{L}$ as the *Liouville operator*. It is not difficult to see that condition 5.2 now gives us the operator identities $\mathcal{P}\mathcal{L}\mathcal{P} = 0$, $\mathcal{Q}\mathcal{L}\mathcal{P} = \mathcal{L}\mathcal{P}$ and $\mathcal{P}\mathcal{L}\mathcal{Q} = \mathcal{P}\mathcal{L}$. These will be used at several occasions in this chapter.

The next thing we do, is to define two different time development operators. These are $G_{t\to t'}$ and $\mathcal{G}_{t\to t'}$. G is the actual time development operator of the total system T. It is given by $G_{t\to t'}\rho_T = U(t,t')\rho_T U^\dagger(t,t')$, and in the interaction picture it obeys the differential equation $\dot{G} = \mathcal{L}G$. $\mathcal{G}$ on the other hand, we define to obey the slightly modified differential equation $\dot{\mathcal{G}} = \mathcal{Q}\mathcal{L}\mathcal{G}$. Like G it is also subject to the initial condition $\mathcal{G}_{t\to t} = \mathcal{I}$.

With these definitions in place we are finally ready to write down the Nakajima Zwanzig equation. We will formulate the equation in terms of the operator $\mathcal{P}\rho_T$. Note however that there is a bijective relationship between $\mathcal{P}\rho_T$ and ρ_S by the relations $\mathcal{P}\rho_T = \rho_S \otimes \rho_E(0)$ and $\rho_S = \mathrm{Tr}_E\mathcal{P}\rho_T$. This means that the Nakajima Zwanzieg equation can easily be reformulated as an equation for ρ_S.

Theorem 3. Nakajima Zwanzig equation.

Let T be a closed quantum system consisting of two subsystems S and E, so that $\mathcal{H}_\mathcal{T} = \mathcal{H}_S \otimes \mathcal{H}_E$. Let the state operators $\rho_T(t)$ of T have a unitary time development which *in the interaction picture* is given by the equation $\dot{\rho}_T = \mathcal{L}\rho_T$, where the Liouville operator $\mathcal{L}(t)$ is defined above. Assume further that at $t = 0$ ρ_T factorizes as $\rho_T(0) = \rho_S(0) \otimes \rho_E(0)$, which can obviously be reexpressed as $\rho_T(0) = \mathcal{P}\rho_T(0)$. Then still in the interaction picture, the operator $\mathcal{P}\rho_T(t) = \rho_S(t) \otimes \rho_E(0)$ will be a solution to *the Nakajima Zwanzieg equation*:

$$\frac{d}{dt}\mathcal{P}\rho_T(t) = \int_0^t \mathcal{K}(t,t')\mathcal{P}\rho_T(t')dt', \tag{5.4}$$

where the memory kernel $\mathcal{K}(t,t')$ is given by

$$\mathcal{K}(t,t') = \mathcal{P}\mathcal{L}(t)\mathcal{G}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}. \tag{5.5}$$

The involved operators $\mathcal{P}$, $\mathcal{L}$, $\mathcal{G}_{t'\to t}$ and $\mathcal{Q}$ are all defined above.

Proof. The derivation is based on one that is found in [2]: In the interaction picture the total system T obeys as mentioned the equation $\dot{\rho}_T = -\frac{i}{\hbar}[H_{SE}, \rho_T] = \mathcal{L}\rho_T$. By applying the two super operators $\mathcal{P}$ and $\mathcal{Q}$ to this equation, we end up with the two equations

$$\frac{d}{dt}\mathcal{P}\rho_T = \mathcal{P}\mathcal{L}\rho_T = \mathcal{P}\mathcal{L}\mathcal{P}\rho_T + \mathcal{P}\mathcal{L}\mathcal{Q}\rho_T, \tag{5.6}$$

$$\frac{d}{dt}\mathcal{Q}\rho_T = \mathcal{Q}\mathcal{L}\rho_T = \mathcal{Q}\mathcal{L}\mathcal{Q}\rho_T + \mathcal{Q}\mathcal{L}\mathcal{P}\rho_T, \tag{5.7}$$

which can be interpreted as coupled linear equations for the two operators $\mathcal{P}\rho_T$ and $\mathcal{Q}\rho_T$. The second of these can be solved to give

$$\mathcal{Q}\rho_T = \int_0^t \mathcal{G}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}\rho_T(t')dt'. \tag{5.8}$$

To verify that this is indeed a solution, we first note that it has the correct initial value, since $\mathcal{Q}\rho_T(0) = \rho_T(0) - \mathcal{P}\rho_T(0) = \rho_S(0)\otimes\rho_E(0) - (\mathrm{Tr}_E\,\rho_T(0))\otimes\rho_E(0) = 0$. Secondly, we differentiate to get

$$\begin{aligned}\frac{d}{dt}\mathcal{Q}\rho_T &= \frac{d}{dt}\int_0^t \mathcal{G}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}\rho_T(t')dt' = \int_0^t \dot{\mathcal{G}}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}\rho_T(t')dt' + \mathcal{G}_{t\to t}\mathcal{Q}\mathcal{L}(t)\mathcal{P}\rho_T(t)\\ &= \int_0^t \mathcal{Q}\mathcal{L}\mathcal{G}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}\rho_T(t')dt' + \mathcal{Q}\mathcal{L}\mathcal{P}\rho_T = \mathcal{Q}\mathcal{L}\mathcal{Q}\rho_T + \mathcal{Q}\mathcal{L}\mathcal{P}\rho_T.\end{aligned} \tag{5.9}$$

This solution can then be inserted in the first equation, which results in the equation

$$\frac{d}{dt}\mathcal{P}\rho_T = \mathcal{P}\mathcal{L}\mathcal{P}\rho_T + \int_0^t \mathcal{P}\mathcal{L}(t)\mathcal{G}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}\rho_T(t')dt' = \int_0^t \mathcal{P}\mathcal{L}(t)\mathcal{G}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}\rho_T(t')dt', \tag{5.10}$$

where the identity $\mathcal{P}\mathcal{L}\mathcal{P} = 0$ has been used. □

As mentioned, one can easily reformulate 5.4 in terms of ρ_S. This equation would then be an exact memory equation for this operator, in the sense that it is equivalent to 3.2. However, whereas 3.2 would involve solving the Schrödinger equation of the total system T, 5.4 equation has the advantage of not explicitly containing any environmental degrees of freedom. This advantage is however far from as big as it might seem, since in order to apply it we would have to find an explicit expression for the memory kernel $\mathcal{K}(t,t')$. This would involve calculating the super operator $\mathcal{G}_{t\to t'}$ by solving the equation $\dot{\mathcal{G}} = \mathcal{Q}\mathcal{L}\mathcal{G}$. Obviously this equation still involves the environmental degrees of freedom, and can be expect to be just as difficult to solve as the Schrödinger equation.

It would seem then that we have not at all gained particularly much by deriving the Nakajima Zwanzig equation, but this is not quite the case: Even though the equation it self is in most cases not practically applicable, it is still an important theoretical tool. Primarily this is as a starting point for the rigorous derivation of approximation schemes that are in fact practically applicable. This will be exemplified in the following sections.

5.2 Perturbative expansion of the Memory kernel

An obvious solution to the problem of finding the super operator $\mathcal{G}_{t\to t'}$, is to simply make a perturbative expansion of it. $\mathcal{G}_{t\to t'}$ satisfies the equation $\dot{\mathcal{G}} = \mathcal{Q}\mathcal{L}\mathcal{G}$, and the initial condition $\mathcal{G}_{t\to t} = \mathcal{I}$. This means it can be expanded in pretty much the same way as the unitary time development operator $U(t)$ is expanded in standard time dependent perturbation theory: We integrate the differential equation to get the integral equation

$$\mathcal{G}_{t\to t'} = I + \int_t^{t'} \mathcal{Q}\mathcal{L}(s)\mathcal{G}_{t\to s}ds. \tag{5.11}$$

Note that this equation defines an expression for $\mathcal{G}_{t\to s}$ which can be inserted on its own right hand side. If we iterate this procedure a total of N times we get

$$\begin{aligned}\mathcal{G}_{t\to t'} =& \sum_{n=0}^{N} \int_t^{t'} \int_t^{t_1} \cdots \int_t^{t_{n-1}} \mathcal{QL}(t_1)\cdots\mathcal{QL}(t_n) dt_n \cdots dt_1 \\ &+ \int_t^{t'} \int_t^{t_1} \cdots \int_t^{t_{n-1}} \mathcal{QL}(t_1)\cdots\mathcal{QL}(t_n)\mathcal{G}_{t\to t_n} dt_n \cdots dt_1. \end{aligned} \tag{5.12}$$

Assuming that the last term approaches 0 as $N \to \infty$ (which is the condition for convergence), then $\mathcal{G}_{t\to t'}$ can be expressed as the infinite series

$$\mathcal{G}_{t\to t'} = \sum_{n=0}^{\infty} \int_t^{t'} \int_t^{t_1} \cdots \int_t^{t_{n-1}} \mathcal{QL}(t_1)\cdots\mathcal{QL}(t_n) dt_n \cdots dt_1. \tag{5.13}$$

This expression can be inserted in 5.5 to give

$$\mathcal{K}(t,t') = \sum_{n=0}^{\infty} \int_{t'}^{t} \int_{t'}^{t_1} \cdots \int_{t'}^{t_{n-1}} \mathcal{PL}(t)\mathcal{QL}(t_1)\cdots\mathcal{QL}(t_n)\mathcal{QL}(t')\mathcal{P} dt_n \cdots dt_1, \tag{5.14}$$

an expression that can be truncated at any n to give a practically calculable approximation. In particular, if we include only the $n = 0$ term we find

$$\begin{aligned}\mathrm{Tr}_E \mathcal{K}(t,t')\mathcal{P}\rho_T(t') &= \mathrm{Tr}_E \mathcal{L}(t)\mathcal{QL}(t')\left(\rho_S(t')\otimes\rho_E(0)\right) = \mathrm{Tr}_E \mathcal{L}(t)\mathcal{QL}(t')\mathcal{P}\left(\rho_S(t')\otimes\rho_E(0)\right) \\ &= \mathrm{Tr}_E\left(\mathcal{L}(t)\mathcal{L}(t')\left(\rho_S(t')\otimes\rho_E(0)\right)\right), \end{aligned} \tag{5.15}$$

where the identity $\mathcal{QLP} = \mathcal{LP}$ has been used. This expression can be seen to be identical to the integrand in 4.28, so that this equation would be reproduced if the $n = 0$ term was all we included in 5.4. This means that 4.28, our first encounter of a memory equation can in fact be interpreted as the lowest order approximation to the Nakajima Zwanzieg equation.

Whenever we express some object using a perturbative expansion like 5.14, we should ask our selves what is the conditions for this expression to be useful. That is to say, essentially what we are wondering is under what conditions the expansion converges after a relatively small n. The usual assumption is that this will be the case when one has a sufficiently small 'smallness parameter'. That is, the parameter who's order increases for each term. In 5.14 we see that each term contains a larger number of Liouville operators $\mathcal{L}(t)$, so that we could take the smallness parameter to be proportional to these. The Liouville operators are again expressed using the interaction operators $\mathcal{H}_{SE}$, so that in fact we can take the smallness parameter to be proportional to the interaction strength.

We thus conclude that 5.14 becomes useful when we have relatively weak interactions. This however introduces a new question: We could also attempt to find the development of $\rho(t)$ by using standard time dependent perturbation theory of the time development operator $U(t)$ of the total system T. This method, which is one of the standard techniques for approximating the development of interacting quantum systems, *also* works best when the interactions are weak. It then initially seems we would gain little by using 5.14 together with 5.4 instead of simply employing standard perturbation theory. This is particularly the case since in applying standard perturbation theory we would not have to solve any additional complicated integro differential equations like 5.4.

So why then would we claim 5.14 to be useful? Well, the story is actually a bit more complicated. Something we completely forgot to consider in the preceding discussion is how the convergence of the expansion *varies with time*. Standard perturbation theory works best for relatively short times t. The reason for this is that the error of the expression in general will increase approximately as t^n. 5.14 however, is based on the expansion 5.13. The error of that expansion is seen from 5.12 to be an integral over an n-dimensional simplex with sides of length $t - t'$, and thus it should increase with $(t - t')^n$. In fact, since

one will get the standard perturbation expression for $U(t)$ from 5.12 by simply making the substitutions $\mathcal{G}_{t\to t'} \to U(t)$, $t' \to t$, $t \to 0$ and $\mathcal{QL} \to H_{SE}$, this also shows that the error of U grows like t^n as stated.

Since 5.14 is found by inserting 5.13 in 5.5, the error of this expression clearly also grows like $(t-t')^n$. This means that as opposed to standard perturbation theory, it is not whether t is small or large that matters to the usefulness of the method, but instead in what range of t and t' the major contribution to the integral in 5.4 comes from: If $\mathcal{K}(t,t')$ is very small in all regions except where t and t' are close, then we can expect good convergence irrespectively of the values these parameters have individually. Thus we may conclude that the advantage of the perturbation method discussed in this section to the standard method, is that the region of fast convergence is not limited to short times.

The convergence will however as mentioned be strongly affected by the t, t' region where $\mathcal{K}(t,t')$ is significantly large. We should discuss this in some detail: Let us assume that $\mathcal{K}(t,t')$ is by a significant amount largest in a region where $|t-t'| < \tau$, that is we assume $\mathcal{K}(t,t')$ to be damped over some characteristic time scale τ which could be interpreted as the effective length of the systems memory. With this assumption, the condition for having fast convergence in applying 5.14 can be formulated simply as the requirement that τ should be sufficiently small.

Small when compared to what? Well if we insert 5.14 in 5.4, then upon examining the terms it seems that each integration should contribute a factor proportional to $V/\hbar \cdot \tau$, where V is some characteristic interaction strength of H_{SE}. Since each new term contains one more such integration this means that the resulting expansion is in fact an expansion in this dimensionless parameter. We thus conclude that we have fast convergence when τ is sufficiently small compared to $\hbar/V$. In standard perturbation theory we can use a similar argument to argue that it is in fact t that must be small compared to $\hbar/V$, again pointing out how the convergence of that method is highly time sensitive.

Another way to formulate this is as follows: I mentioned above that both of the two perturbation methods are best in the weak interaction limit. We see now that this is true, but also that there is a difference in the explicit condition: standard perturbation theory works best when the interactions are weak in comparison to $\hbar/t$, while the expansion of the memory kernel works when they are weak in comparison to $\hbar/\tau$. Now, in [2] and [1] it is claimed that $\tau \sim \hbar/\Delta E$, with ΔE being a characteristic width of the energy spectrum of the environment E. I will make no attempt to show that this is true in general, but I will demonstrate that it is indeed the case when dealing with a specific example: the two level model. This will be done in the next chapter, where it will be a major point. In any case, this means that the condition for quick convergence of the memory kernel expansion is simply that V must be sufficiently small when compared to ΔE.

As long as this is the case, and we are dealing with dynamics that are truly non-Markovian, this expansion seems in fact like the best way of treating open systems. Provided of course that we have a believable unitary model of the total system T, and that this is to difficult to solve exactly. However, as I have mentioned at several occasions: open system are in fact often *not* truly non-Markovian, since it is in principle possible to find a Markovian generator that describes them exactly. In these cases it seems like somewhat of an overkill to use complicated integro-differential equations like 5.4. Instead it would be nice if we could somehow approximate the Markovian generator, since we could then treat the problem using just normal differential equations. In the last section of this chapter I will show that such an approximation scheme actually do exist, but first I will spend a section on the discussion of the exact generator itself.

5.3 Exact Markovian equation

In section 4.2 I tried to argue that under certain assumptions Markovianness is equivalent to the invertibility of the time development operators. I also demonstrated that even without these assumptions, such invertibility certainly implies Markovianness. So let us now assume that we have some general linear

integro-differential equation

$$\dot{x} = \int_0^t \mathcal{K}(t,t')x(t')dt' \tag{5.16}$$

that defines a time development operator $g(t)$ that is left invertible. Then according to the arguments of section 4.2, the development of $x(t)$ should be Markovian. Since it in this case is clearly also differentiable, there should exist some Markovian generator $\mathcal{M}(t)$ that describes the system through the equation $\dot{x} = \mathcal{M}(t)x$. Can we find an expression for this generator in terms of the previously encountered operators? Yes. It is in fact easily seen that this can be done, and that the expression is simply

$$\mathcal{M}(t) = \int_0^t \mathcal{K}(t,t')g(t')dt'g^{-1}(t) = \int_0^t \mathcal{K}(t,t')g_{t\to t'}dt', \tag{5.17}$$

where we have again defined $g_{t\to t'} = g(t')g^{-1}(t)$. That this is indeed the Markovian generator can be verified by simply inserting the expression in $\dot{x} = \mathcal{M}(t)x$, and comparing with 5.16.

Specializing to our topic of interest: open quantum systems, the discussion remains essentially the same. The differences being just that x is replaced with ρ, and that $\mathcal{K}(t,t')$ is now the (exact) Nakajima Zwanzieg kernel. In particular 5.17 remains as it stands. However, this exact expression for the Markovian generator is not practically applicable: First of all it involves the exact Nakajima Zwanzieg kernel, which is it self not explicitly calculable. This problem was however dealt with in the previous section. A problem that is much bigger, is that the expression involves the operators $g(t)$ and $g^{-1}(t)$, which are clearly unknown. In fact, had we known any of these operators the problem of interest would already be solved.

Thus, the only usefulness of 5.17 lies in taking it as a starting point for some approximation scheme. Truth to be told, [2] which is my primary source on this topic, does not even mention this equation. And neither does any other sources I have seen. In [2] there is however derived an expansion of the Markovian generator, which to the highest explicitly calculated order can be seen to be identical to the one I will derive from 5.17 in the next section. In [2] a completely different starting point is used for deriving this expansion: There it is shown that the exact Markovian generator is given by the expression

$$\mathcal{M}(t)\rho_S(t) = \mathrm{Tr}_E\mathcal{L}(t)(1-\Sigma(t))^{-1}\rho_S(t)\otimes\rho_E(0), \tag{5.18}$$

where the operator $\Sigma(t)$ is defined as

$$\Sigma(t) = \int_0^t \mathcal{G}_{t'\to t}\mathcal{Q}\mathcal{L}(t')\mathcal{P}G_{t\to t'}dt', \tag{5.19}$$

and it is assumed that $1-\Sigma(t)$ is invertible. Clearly, it must be possible to derive this from 5.17, but it is in fact far easier to derive it directly from the equations 5.6 and 5.7, which is what is done in [2]. Here however we shall do neither, since we will in fact not have any need for this expression. My starting point will instead be 5.17, together with a perturbation expansion of $g_{t\to t'}$.

5.4 Perturbative expansion of the Markovian generator

Clearly, the super operator $g(t)$ must satisfy the equation

$$\dot{g}(t) = \int_0^t \mathcal{K}(t,t')g(t')dt', \tag{5.20}$$

since then $x(t) = g(t)x(0)$ will satisfy 5.16. It is then easily seen that as long as $g^{-1}(t)$ exists, the operator $g_{s\to t} = g(t)g^{-1}(s)$ must satisfy essentially the same equation:

$$\dot{g}_{s\to t} = \dot{g}(t)g^{-1}(s) = \int_0^t \mathcal{K}(t,t')g(t')dt'g^{-1}(s) = \int_0^t \mathcal{K}(t,t')g_{s\to t'}dt', \tag{5.21}$$

independently of whether $s < t$. This equation may be integrated to give

$$g_{s\to t} = I + \int_s^t \int_0^r \mathcal{K}(r,t')g_{s\to t'}dt'dr, \tag{5.22}$$

an expression that may be iterated in the standard fashion of perturbation theory to give

$$g_{s\to t} = \sum_{n=0}^{\infty} \int_s^t \int_0^{r_1} \int_s^{t_1} \cdots \int_s^{t_{n-1}} \int_0^{r_n} \mathcal{K}(r_1,t_1)\cdots\mathcal{K}(r_n,t_n)dt_n dr_n \cdots dt_1 dr_1, \tag{5.23}$$

provided of course that the series converges. This expression may then be inserted in 5.17 to finally give

$$\mathcal{M}(t) = \sum_{n=0}^{\infty} \int_0^t \int_t^{t'} \int_0^{t_1} \int_t^{t'_1} \cdots \int_t^{t'_{n-1}} \int_0^{t_n} \mathcal{K}(t,t')\mathcal{K}(t_1,t'_1)\cdots\mathcal{K}(t_n,t'_n)dt'_n dt_n \cdots dt'_1 dt_1 dt'. \tag{5.24}$$

This equation is a general expansion of the Markovian generator of any equation on the form 5.16 where the development is invertible. We will soon turn to specializing this to the theory of open quantum systems, but first we will again discuss the parameter ranges in which this expansion is useful: In much the same way as was done in section 5.2, one can argue that low n truncations of 5.23 will be justified when the contributing t_i are all close to s. In order for this to be the case, t must be close to s, and secondly the kernel $\mathcal{K}(r,t)$ must be quickly damped when r departs from t.

For truncations of 5.24 to be justified, it is then easily seen that precisely the same conditions are needed: $\mathcal{K}(t,t')$ must be quickly damped, and the contributing t' must be close to t. The later will however be a consequence of the rapid damping of $\mathcal{K}(t,t')$, so that this is in fact the only condition for truncations to be good approximations. Note also that this is in fact the same condition that was found for truncations of the memory kernel expansion 5.14 to be valid.

Let us now return the discussion of Markovian generators to the subject of the thesis: open quantum systems. The easiest way of doing this, is to order by order insert the expansion 5.15 of the memory kernel into the expansion 5.24 of the Markovian generator. It is difficult to write down the general result, but it is easy to find concrete terms to a quite high order in the Liouville operators $\mathcal{L}(t)$. To illustrate this I will find all terms to the sixth order. The reader should be warned that the following will be fairly technical.

Let us denote the n'th order term of $\mathcal{M}(t)$ by $\mathcal{M}_n(t)$ and the nth order term of $\mathcal{K}(t,t')$ by $\mathcal{K}_n(t,t')$. From 5.24 we then have to the sixth order

$$\begin{aligned}
\mathcal{M}(t) =& \mathcal{M}_2(t) + \mathcal{M}_3(t) + \mathcal{M}_4(t) + \mathcal{M}_5(t) + \mathcal{M}_6(t) + \cdots \\
=& \int_0^t \mathcal{K}_2(t,t') + \mathcal{K}_3(t,t') + \mathcal{K}_4(t,t') + \mathcal{K}_5(t,t') + \mathcal{K}_6(t,t') + \cdots dt' \\
&+ \int_0^t \int_t^{t'} \int_0^{t_1} \left(\mathcal{K}_2(t,t') + \mathcal{K}_3(t,t') + \mathcal{K}_4(t,t')\cdots\right)\left(\mathcal{K}_2(t_1,t'_1) + \mathcal{K}_3(t_1,t'_1) + \mathcal{K}_4(t_1,t'_1)\cdots\right) dt'_1 dt_1 dt' \\
&+ \int_0^t \int_t^{t'} \int_0^{t_1} \int_t^{t'_1} \int_0^{t_2} \left(\mathcal{K}_2(t,t') + \cdots\right)\left(\mathcal{K}_2(t_1,t'_1) + \cdots\right)\left(\mathcal{K}_2(t_2,t'_2) + \cdots\right) dt'_2 dt_2 dt'_1 dt_1 dt' + \cdots \\
=& \int_0^t \mathcal{K}_2(t,t') + \mathcal{K}_3(t,t') + \mathcal{K}_4(t,t') + \mathcal{K}_5(t,t') + \mathcal{K}_6(t,t') + \cdots dt' \\
&+ \int_0^t \int_t^{t'} \int_0^{t_1} \mathcal{K}_2(t,t')\mathcal{K}_2(t_1,t'_1) + \mathcal{K}_2(t,t')\mathcal{K}_3(t_1,t'_1) + \mathcal{K}_3(t,t')\mathcal{K}_2(t_1,t'_1) \\
&+ \mathcal{K}_2(t_1,t'_1)\mathcal{K}_4(t_1,t'_1) + \mathcal{K}_4(t,t')\mathcal{K}_2(t_1,t'_1) + \mathcal{K}_3(t,t')\mathcal{K}_3(t_1,t'_1) + \cdots \; dt'_1 dt_1 dt' \\
&+ \int_0^t \int_t^{t'} \int_0^{t_1} \int_t^{t'_1} \int_0^{t_2} \mathcal{K}_2(t,t')\mathcal{K}_2(t_1,t'_1)\mathcal{K}_2(t_2,t'_2) + \cdots dt'_2 dt_2 dt'_1 dt_1 dt' + \cdots
\end{aligned} \tag{5.25}$$

Collecting terms of the same order, we find

$$\mathcal{M}_2(t) = \int_0^t \mathcal{K}_2(t,t')dt' \tag{5.26}$$

$$\mathcal{M}_3(t) = \int_0^t \mathcal{K}_3(t,t')dt' \tag{5.27}$$

$$\mathcal{M}_4(t) = \int_0^t \mathcal{K}_4(t,t')dt' + \int_0^t \int_t^{t'} \int_0^{t_1} \mathcal{K}_2(t,t')\mathcal{K}_2(t_1,t_1')dt_1'dt_1dt' \tag{5.28}$$

$$\mathcal{M}_5(t) = \int_0^t \mathcal{K}_5(t,t')dt' + \int_0^t \int_t^{t'} \int_0^{t_1} \mathcal{K}_2(t,t')\mathcal{K}_3(t_1,t_1') + \mathcal{K}_3(t,t')\mathcal{K}_2(t_1,t_1')dt_1'dt_1dt' \tag{5.29}$$

$$\begin{aligned}\mathcal{M}_6(t) = &\int_0^t \mathcal{K}_6(t,t')dt' \\ &+ \int_0^t \int_t^{t'} \int_0^{t_1} \mathcal{K}_2(t,t')\mathcal{K}_4(t_1,t_1') + \mathcal{K}_4(t,t')\mathcal{K}_2(t_1,t_1') + \mathcal{K}_3(t,t')\mathcal{K}_3(t_1,t_1')dt_1'dt_1dt' \\ &+ \int_0^t \int_t^{t'} \int_0^{t_1} \int_t^{t_1'} \int_0^{t_2} \mathcal{K}_2(t,t')\mathcal{K}_2(t_1,t_1')\mathcal{K}_2(t_2,t_2')dt_2'dt_2dt_1'dt_1dt'\end{aligned} \tag{5.30}$$

From 5.15 we also see that

$$\mathcal{K}_2(t,t') = \mathcal{PL}(t)\mathcal{QL}(t')\mathcal{P} \tag{5.31}$$

$$\mathcal{K}_3(t,t') = \int_{t'}^t \mathcal{PL}(t)\mathcal{QL}(t_1)\mathcal{QL}(t')\mathcal{P}dt_1 \tag{5.32}$$

$$\mathcal{K}_4(t,t') = \int_{t'}^t \int_{t'}^{t_1} \mathcal{PL}(t)\mathcal{QL}(t_1)\mathcal{QL}(t_2)\mathcal{QL}(t')\mathcal{P}dt_2dt_1 \tag{5.33}$$

$$\mathcal{K}_5(t,t') = \int_{t'}^t \int_{t'}^{t_1} \int_{t'}^{t_2} \mathcal{PL}(t)\mathcal{QL}(t_1)\mathcal{QL}(t_2)\mathcal{QL}(t_3)\mathcal{QL}(t')\mathcal{P}dt_3dt_2dt_1 \tag{5.34}$$

$$\mathcal{K}_6(t,t') = \int_{t'}^t \int_{t'}^{t_1} \int_{t'}^{t_2} \int_{t'}^{t_3} \mathcal{PL}(t)\mathcal{QL}(t_1)\mathcal{QL}(t_2)\mathcal{QL}(t_3)\mathcal{QL}(t_4)\mathcal{QL}(t')\mathcal{P}dt_4dt_3dt_2dt_1. \tag{5.35}$$

Inserting this in the equations 5.26 to 5.30 and applying the identities $\mathcal{QLP} = \mathcal{LP}$ and $\mathcal{PLQ} = \mathcal{PL}$ we finally get

$$\mathcal{M}_2(t) = \int_0^t \mathcal{PL}(t)\mathcal{L}(t')\mathcal{P}dt' \tag{5.36}$$

$$\mathcal{M}_3(t) = \int_0^t \int_{t'}^t \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{L}(t')\mathcal{P}dt_1dt' \tag{5.37}$$

$$\begin{aligned}\mathcal{M}_4(t) = &\int_0^t \int_{t'}^t \int_{t'}^{t_1} \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{L}(t')\mathcal{P}dt_2dt_1dt' \\ &+ \int_0^t \int_t^{t'} \int_0^{t_1} \mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}dt_1'dt_1dt'\end{aligned} \tag{5.38}$$

$$\mathcal{M}_5(t) = \int_0^t \int_{t'}^t \int_{t'}^{t_1} \int_{t'}^{t_2} \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{QL}(t_3)\mathcal{L}(t')\mathcal{P}dt_3dt_2dt_1dt'$$

$$+\int_0^t\int_t^{t'}\int_0^{t_1}\int_{t_1'}^{t_1}\mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(\bar{t}_1)\mathcal{L}(t_1')\mathcal{P}d\bar{t}_1dt_1'dt_1dt'$$

$$+\int_0^t\int_t^{t'}\int_0^{t_1}\int_{t'}^{t}\mathcal{PL}(t)\mathcal{L}(\bar{t}_1)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}d\bar{t}_1dt_1'dt_1dt' \tag{5.39}$$

$$\begin{aligned}\mathcal{M}_6(t) =& \int_0^t\int_{t'}^t\int_{t'}^{t_1}\int_{t'}^{t_2}\int_{t'}^{t_3}\mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{QL}(t_3)\mathcal{QL}(t_4)\mathcal{L}(t')\mathcal{P}dt_4dt_3dt_2dt_1dt'\\
&+\int_0^t\int_t^{t'}\int_0^{t_1}\int_{t_1'}^{t_1}\int_{t_1'}^{\bar{t}_1}\mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(\bar{t}_1)\mathcal{QL}(\bar{t}_2)\mathcal{L}(t_1')\mathcal{P}d\bar{t}_2d\bar{t}_1dt_1'dt_1dt'\\
&+\int_0^t\int_t^{t'}\int_0^{t_1}\int_{t'}^{t}\int_{t'}^{\bar{t}_1}\mathcal{PL}(t)\mathcal{L}(\bar{t}_1)\mathcal{QL}(\bar{t}_2)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}d\bar{t}_2d\bar{t}_1dt_1'dt_1dt'\\
&+\int_0^t\int_t^{t'}\int_0^{t_1}\int_{t'}^{t}\int_{t_1'}^{t_1}\mathcal{PL}(t)\mathcal{L}(\bar{t}_1)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(\bar{\bar{t}}_1)\mathcal{L}(t_1')\mathcal{P}d\bar{\bar{t}}_1d\bar{t}_1dt_1'dt_1dt'\\
&+\int_0^t\int_t^{t'}\int_0^{t_1}\int_{t}^{t_1'}\int_{0}^{t_2}\mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_2)\mathcal{L}(t_1')\mathcal{PL}(t_2)\mathcal{L}(t_2')\mathcal{P}dt_2'dt_2dt_1'dt_1dt'.\end{aligned} \tag{5.40}$$

Quite often the identity $\mathcal{PLP}=0$ can be extended to similar expressions involving any odd number of $\mathcal{L}$s. In that case $\mathcal{M}_3$ and $\mathcal{M}_5$ would be zero just like $\mathcal{M}_1$.

If we truncate the expansion already after the lowest order term $\mathcal{M}_2$, the Markovian equation for ρ_S becomes

$$\dot{\rho}_S = \mathrm{Tr}_E\mathcal{M}_2(\rho_S\otimes\rho_E(0)) = \mathrm{Tr}_E\left(\int_0^t\mathcal{L}(t)\mathcal{L}(t')dt'(\rho_S\otimes\rho_E(0))\right). \tag{5.41}$$

If we insert the definition $\mathcal{L}(t)\rho = -i/\hbar\cdot[H,\rho]$ in this, the equation can be seen to be identical to the Redfield equation 4.29. With this we finally have the more rigorous derivation of the Redfield equation that was mentioned in the previous chapter: It is simply the lowest order term in a perturbation expansion of the exact Markovian generator. The expansion 5.25 is best for short memory kernels. In order for it to be a good approximation to include only the lowest order term like this, this memory kernel must be very short indeed. If this is the case, then it is also reasonable to assume that it will be a good approximation to set the upper integral limit to infinity. If this is done, we will once again get 4.30.

In the previous section, I mentioned that an expansion of the form 5.36 is derived also in [2]. There however with a slightly different starting point. Obviously this expansion should be compared with the one I have found my self. Actually, in [2] the calculation is only done to the 4. order, so that obviously this will be the highest order to which the comparison can be made. To that order the expressions are in fact completely identical, but in order to see this we must first rewrite the third and fourth order terms:

It is not hard to convince one self that in general

$$\int_0^a\int_y^a f(x,y)dxdy = \int_0^a\int_0^x f(x,y)dydx. \tag{5.42}$$

Both integrals simply expresses a 2 dimensional integral over a triangle with corners in (0,0), (0,a) and (a,a). This can be applied directly to 5.37 to get

$$\mathcal{M}_3(t) = \int_0^t\int_0^{t_1}\mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{L}(t')\mathcal{P}dt'dt_1. \tag{5.43}$$

5.42 can also be used to rewrite 5.38, though this is not quite as straight forward:

$$\begin{aligned}
\mathcal{M}_4(t) &= \int_0^t \int_{t'}^t \int_{t'}^{t_1} \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{L}(t')\mathcal{P}dt_2dt_1dt' + \int_0^t \int_t^{t'} \int_0^{t_1} \mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}dt_1'dt_1dt' \\
&= \int_0^t \int_0^{t_1} \int_{t'}^{t_1} \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{L}(t')\mathcal{P}dt_2dt'dt_1 - \int_0^t \int_0^{t_1} \int_0^{t_1} \mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}dt_1'dt'dt_1 \\
&= \int_0^t \int_0^{t_1} \int_0^{t_2} \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{L}(t')\mathcal{P}dt'dt_2dt_1 - \int_0^t \int_0^{t_1} \int_0^{t'} \mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}dt_1'dt'dt_1 \\
&\quad - \int_0^t \int_0^{t_1} \int_{t'}^{t_1} \mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}dt_1'dt'dt_1 \\
&= \int_0^t \int_0^{t_1} \int_0^{t_2} \mathcal{PL}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{L}(t')\mathcal{P} - \mathcal{PL}(t)\mathcal{L}(t_2)\mathcal{PL}(t_1)\mathcal{L}(t')\mathcal{P}dt'dt_2dt_1 \\
&\quad - \int_0^t \int_0^{t_1} \int_0^{t'} \mathcal{PL}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_1')\mathcal{P}dt'dt_1'dt_1 \\
&= \int_0^t \int_0^{t_1} \int_0^{t_2} \mathcal{P}\left(\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{QL}(t_2)\mathcal{L}(t') - \mathcal{L}(t)\mathcal{L}(t_2)\mathcal{PL}(t_1)\mathcal{L}(t') - \mathcal{L}(t)\mathcal{L}(t')\mathcal{PL}(t_1)\mathcal{L}(t_2)\right)\mathcal{P}dt'dt_2dt_1
\end{aligned} \tag{5.44}$$

5.43 and 5.44 can be seen to be completely identical to the third and fourth order expressions found in [2]. Also, 5.36 is identical to the second order expression in [2], without any need of rewriting. This clearly indicates that this method is equivalent to the one applied there.

Finally, I should say some words concerning the reason why I use this method to find the perturbation expansion instead of the one applied in [2]. Well, first of all it is simply because I find this method simpler, more direct and less cumbersome. Secondly, when using this method it is easier to see that the existence of Markovian expansions like this is not something that is limited to the theory of open quantum systems: As mentioned in section 5.3, any system that is described by a memory equation on the form 5.16 and has an invertible time development has an exact Markovian generator that can be expanded as 5.24. In fact, it is this expression that will be employed in this thesis. 5.36 to 5.40 was only calculated to show that this method can be applied very generally.

When using this method it is also possible to stress that it is the damping time τ of the memory kernel that determines the convergence, and not the time t since initialization. This is harder when using the method in [2], since this makes an expansion around the initial time $t = 0$. Finally, when taking 5.17 as the starting point of the expansion, it becomes clear that it is the invertibility of the time development operator $g(t)$ that is the necessary requirement. As was discussed in 4.2 this is under quite believable conditions a requirement of Markovianness in any case. In addition, invertibility of these operators were found to be a justifiable assumption in many cases, at least in some finite interval. When starting instead with 5.18 as in [2] however, it is the operator $1 - \Sigma(t)$ that must be invertible. Due to the somewhat abstract definition of this operator it is difficult to see whether this is a believable assumption, and how it connects with Markovianness in general.

Part II

Concrete models

Chapter 6

Decay of a two-level system

6.1 Description of the model

The first example of an open system I will treat is one of the simplest one imaginable: To obtain this we choose for the system S the simplest possible quantum mechanical object, the two-level system, and we couple it to one of the simplest possible environments, namely a bath of harmonic oscillators. To make the model even simpler we assume the bath to initially be in the vacuum state.

Now, this being such a simple model one might wonder whether it actually describes anything useful. The answer turns out to be that it does. Those already familiar with some quantum mechanics will recognize this as the model that is normally used to describe the decay of some high energy physical state into a lower one. For instance this could be an excited atom emitting a photon to fall into its ground state, or a radioactive nuclei emitting some kind of radiation to decay into a lighter isotope.

Let us describe the model in detail: We denote the two-level system S and the bath E. Let the two levels of S, $|g\rangle$ and $|e\rangle$ have energies 0 and E_0 respectively. Let σ_+ be the raising operator and P_i the projection operator on the state i. Further, we let E consist of a set of oscillators indexed by k. The frequency of the oscillators are ω_k, and we name the annihilation operators a_k and the number operators N_k. Finally, we write up an expression for the systems Hamiltonian:

$$H = H_S + H_E + H_{SE} = E_0 P_e + \sum_k \hbar\omega_k N_k + \sum_k (w_k a_k \sigma_+ + w_k^\star a_k^\dagger \sigma_-), \tag{6.1}$$

where the interaction terms are contained in H_{SE}. In principle we could also have interactions of the form $a_i\sigma_-$ or $a_i^\dagger\sigma_+$, but in this model we assume that the energy E_0 is large compared to the interaction strength. Interactions on the form $a_i\sigma_-$ or $a_i^\dagger\sigma_+$ correspond to transitions between states with an energy difference of $E_0 + \hbar\omega_k \geq E_0$, which would then be strongly damped. We therefore ignore these terms, an approximation often referred to as the rotating wave approximation[2], because it in the theory of NMR corresponds to replacing linear polarized with circular polarized, or rotating radio waves.

We now further limit our study to the case where the bath is initially in the vacuum state. The interaction above only allows for two types of transfer: exiting S while deexciting the bath, and deexciting S while exiting the bath. Since the system only has two levels this means that if the bath starts out in the vacuum state, it can never contain more than a single excitation. To phrase things more mathematically: if the total system starts out in the subspace of its Hilbert space where either the two-level system is excited and the bath in its vacuum state, or the two-level system is in the ground state and the bath contains one excitation, then it can never leave this subspace. In addition to these states we also include in this subspace the state where both S and E are in the ground state. This state only interacts with itself, and so the subspace is still closed.

Assuming then that we are in this subspace, we can rewrite the Hamiltonian slightly. We now refer to the state where the two-level system is excited and the bath is in vacuum as $|e\rangle$, and the state where they are both in the ground state as $|g\rangle$. The state where the two-level system is in the ground state, oscillator k is in the first excited level and all other oscillators are in the vacuum state we call $|k\rangle$. All vectors in

our subspace can now be expanded as $c\,|e\rangle + c_g\,|g\rangle + \sum_k c_k\,|k\rangle$, while the Hamiltonian can be rewritten

$$H = E_0\,|e\rangle\langle e| + \sum_k \hbar\omega_k\,|k\rangle\langle k| + \sum_k (w_k\,|e\rangle\langle k| + w_k^\star\,|k\rangle\langle e|). \tag{6.2}$$

6.2 Outline of the chapter

As already mentioned this model is used in many texts on quantum mechanics[5][1] to study the decay of a high energy state, and in particular to find an expression for the decay rate. The most common way of performing this analysis is through the use of first order perturbation theory, and this is also where I will start. This will be done in section 6.3. Here we will discuss the behavior of the probability $P(t)$ for remaining in the excited state $|e\rangle$ when t is very small. In connection with this we will also have our first meeting with two important time scales that characterizes this model, and the consequences of whether these time scales are separated. In particular we shall see that the nominal result, known as Fermi's Golden rule relies on such a separation of time scales.

This time scale separation will be seen to be the same one that is required for the Redfield equation described in section 4.4 to be a good approximation. In section 6.4 we will therefore assume that this separation applies and use the Redfield formalism to extend the results of the preceding section beyond very short times. We will see that this formalism results in exponential decay, in agreement with the typical assumption and the experimental observations. We will analyze the system using both 4.29 and 4.30.

I stress again that the Redfield formalism is only valid when there is time scale separation, or equivalently in the limit of weak interactions. We thus still do not have any knowledge of how the decay proceeds over long time scales when this condition is not satisfied. In section 6.5 we will study also these cases by using exact diagonalization. This method however requires us to assume that the environment E only contains a finite number of oscillators. When studying the decay of a two-level system the most realistic assumption is that the oscillators form a continuum. So in this sense the exact diagonalization results are still only approximations, and most interesting in the limit where the energy/frequency spacing between the oscillators goes to 0.

By comparison with the Redfield solutions we shall find that the diagonalization results seem to be largely in agreement with the continuum limit in a time interval of length $2\pi/\delta\omega$, $\delta\omega$ being the frequency spacing between the oscillators. We can then also study the strongly interacting cases in this range, and we find that in contrast to the weakly interacting cases they do not evolve exponentially. In addition do this we will also have a short look at the agreement between the Redfield solution and diagonalization in relation to the shift of energy (Lamb shift) in the two-level system due to the environmental coupling.

In section 6.6 we will study the system using another exact method, namely by the use of an integro differential equation of the type described in chapter 5. We shall however not use the Nakajima Zwanzieg equation, which will instead be delayed to section 6.7. This is because it turns out that this model can be completely described in terms of a simple scalar memory equation with an exactly calculable kernel. That this offers great advantages to the Nakajima Zwanzieg equation should be obvious.

We will use the memory equation approach to study three different questions: First, we will analyze what I have chosen to call the Markovian limit. Here we will see that we can use the memory equation to see very directly why it is that the time scale separation/weak interactions condition leads to an approximate Markovian description and exponential decay. Secondly we will see that when $t \to \infty$ the memory equation sometimes admits exact exponential solutions. This causes us to suspect that these solution will form the asymptotic development of the system, so that we in this asymptotic limit still have exponential decay even when we have strong interactions.

The question of whether this is the case will be treated by numerically analyzing the behavior of the decay for very long times (on the order of 10 life times). This will also be done using the memory equation, which can be solved numerically using a Laplace transform. To increase our faith in these solutions we also compare them with diagonalization results. This will however only be done at modest time scales ($\sim$

4 life times), since it is to numerically demanding to extend the diagonalization solutions to large times without reducing accuracy.

The third subject to be treated using the memory equation approach is in fact precisely the long time behavior of the diagonalization results. As mentioned above these solutions (which are exact if we assume the environment to consist of a finite number of oscillators) only agree with the continuum limit in the interval $[0, 2\pi/\delta\omega]$. After this interval the development completely changes character. In addition it seems that these abrupt changes in behavior repeat them selves with period $\pi/\delta\omega$. We will see that this can be explained by the fact that for the type of oscillator distributions used in the diagonalization, the memory kernel becomes periodic and that the period is precisely this quantity. In the weak interaction limit this periodic memory kernel can be approximated by a sum of delta functions. We will use this to obtain an analytic expression for the development in this limit. This expression will be compared with the diagonalization results.

In section 6.7 we will as mentioned study the system using the Nakajima Zwanzieg equation. This is mainly to check that this is in agreement with the earlier results, as it will not give us any new information about the system. The kernel of the equation will be calculated only to the fourth order.

In section 6.8 we use a Markovian expansion as described in section 5.4. We will however not use the particular generator for the state operator ρ which is described there and is based on the Nakajima Zwanzieg equation. Instead we will apply the same general method to the earlier described scalar memory equation. This greatly reduces the difficulty, and allows us to go to a quite high order by doing some systematic rewritings. The solutions found using this method will be compared with the solutions of the memory equation it self. As this expansion of the generator works for arbitrarily large times, it will also be used to get a second opinion on the asymptotic development.

6.3 Analysis by first order perturbation

In first order perturbation theory we have simple expressions for the transition amplitudes between different states. Let us say the system starts out in state $|i\rangle$, and we want to know the probability amplitude for having the state $|f\rangle$ after some time t. Both $|i\rangle$ and $|f\rangle$ are eigenstates of the non-interacting part H_0 of the Hamiltonian. Then according to the approximation scheme of first order perturbation[5], the amplitude is given by

$$a_{i\to f} = \delta_{if} + \frac{1}{i\hbar}\int_0^t \langle f|\, H_{SE}\, |i\rangle\, e^{i(E_i-E_f)\tau/\hbar} d\tau. \tag{6.3}$$

In our case we are particularly interested in the transition amplitude from the state $|e\rangle$ to one of the states $|k\rangle$. We then need to calculate the quantity $\langle k|\, H_{SE}\, |e\rangle$. It is easily seen from 6.2 that this is simply $w_k^\star$. So we get

$$a_{e\to k} = \frac{1}{i\hbar}\int_0^t w_k^\star e^{i(E_0/\hbar-\omega_k)\tau} d\tau = \frac{w_k^\star}{i\hbar}\frac{e^{i(E_0/\hbar-\omega_k)t}-1}{i(E_0/\hbar-\omega_k)}. \tag{6.4}$$

The probability of transfer is then

$$P_{e\to k} = |a_{e\to k}|^2 = \left(\frac{|w_k|}{\hbar}\right)^2 \frac{2(1-\mathcal{R}e(e^{i(E_0/\hbar-\omega_k)t}))}{(E_0/\hbar-\omega_k)^2} = \left(\frac{|w_k|t}{\hbar}\right)^2 \mathrm{sinc}^2((E_0/\hbar-\omega_k)t/2), \tag{6.5}$$

where we use the sinc function $\mathrm{sinc}\, x = \frac{\sin x}{x}$. Further, the probability of remaining in the $|e\rangle$ state will be

$$P = 1 - \sum_k P_{e\to k} = 1 - \sum_k \left(\frac{|w_k|t}{\hbar}\right)^2 \mathrm{sinc}^2((E_0/\hbar-\omega_k)t/2) = 1 - \left(\frac{t}{\hbar}\right)^2 \int_{-\infty}^{\infty} W(\omega)\mathrm{sinc}^2\frac{\omega t}{2}\, d\omega, \tag{6.6}$$

where we have now made the very important definition

$$W(\omega) = \sum_k |w_k|^2 \delta(\omega - \omega_k + E_0/\hbar), \tag{6.7}$$

which will be used at several different occasions in this chapter. One should note that although this function is defined as a sum of delta functions, one can take the continuum limit in this expression and get a continuous and finite $W(\omega)$. For instance if $W(\omega) = \frac{1}{N}\sum_{n=-\infty}^{\infty}\delta(\omega - \frac{n}{N})$, one can take the limit $N \to \infty$ to get $W(\omega) = 1$ (obviously we have here used dimensionless units). If all environmental states with the same energy $\hbar\omega_k$ also have the same interaction strength $w_k = w(\hbar\omega_k)$, then $W(\omega)$ can be factorized as

$$W(\omega) = \hbar|w(E_0 + \hbar\omega)|^2\mathcal{D}(E_0 + \hbar\omega), \tag{6.8}$$

where $\mathcal{D}(E)$ is the state density function of the environment. Taking this expression in to account, an appropriate name of the function $W(\omega)$ could perhaps be the 'interaction density'. I will however mostly refer to it simply as the 'W function'.

Now back to the expression 6.6. This is a first order perturbation, and as such it applies only for small times t. More precisely it applies when $t \ll \hbar^2/W(0)$. We will come back to the reason for this, but let us first take a look at the expression when we also assume that $t \ll 1/\Delta\omega$, where $\Delta\omega$ is some characteristic width of the function $W(\omega)$. More precisely $\Delta\omega$ is the width of a region around 0 where $W(\omega)$ is significantly larger than outside, which means that the majority of the contribution to the integral in 6.6 comes from ω satisfying $|\omega| < \Delta\omega$. If $t \ll 1/\Delta\omega$ we then have $\omega t \ll 1$ for all contributing ω, so that we can expand the sinc function to get

$$P = 1 - \frac{t^2}{\hbar^2}\int_{-\infty}^{\infty} W(\omega)d\omega. \tag{6.9}$$

For such typically very short times, the occupation probability of the excited state falls of quadratically with time. This could also have been shown directly from the Schrodinger equation in the following way: In the interaction picture the coefficients c_k at $t = 0$ satisfy $\dot{c}_k = \langle k|\dot{\psi}\rangle = -i/\hbar \cdot \langle k| H_{SE} |e\rangle = -iw_k/\hbar$. For very short times then we have $c_k \approx -iw_k t/\hbar$ and $|c_k|^2 \approx |w_k|^2/\hbar^2 \cdot t^2$. Due to conservation of the norm of the state vector we must have $P = |c|^2 = 1 - \sum_k |c_k|^2$, which through the application of 6.7 results in 6.9. This initially quadratic decay is connected to a phenomenon known as the Quantum Zeno Effect[2]. Finally I should also mention that in most applications, such as the theory of decay due to electromagnetic interactions, the integral in 6.9 is actually infinite, and so one must wonder whether there actually is any real region of quadratic decay.

Let us now also look at the opposite limit, where $t \gg q/\Delta\omega$. Since as mentioned 1. order perturbation theory only applies when $t \ll \hbar^2/W(0)$, analyzing this limit would imply that we have a separation of time scales where $\tau_1 = 1/\Delta\omega \ll \tau_2 = \hbar^2/W(0)$. Here $\Delta\omega$ should no longer be interpreted as a characteristic width of W, but rather as the smallest scale over which W varies around 0. That is for all $\omega \ll \Delta\omega$ we have $W(\omega) \approx W(0)$. Note that for simple W functions these two meanings of $\Delta\omega$ should be approximately equal.

An alternative way of formulating this time scale separation is to say that the interaction strength must be weak compared to the energy scale in the environment. Or more specifically that $W(0)/\hbar \ll \Delta E = \hbar\Delta\omega$, where ΔE is the effective width of the environmental energy range that S interacts with. In most physically realistic situations this will be the case. If it is, first order perturbation theory and thus 6.6 still holds in the range $\tau_1 \ll t \ll \tau_2$.

The sinc function in 6.6 has a characteristic width $2/t$. When $\tau_1 \ll t$ we clearly have $2/t \ll \Delta\omega$, so that the only significant contributions to the integral comes from the range where $W(\omega) \approx W(0)$. This means that 6.6 to good accuracy simplifies to

$$P = 1 - \left(\frac{t}{\hbar}\right)^2 W(0)\int_{-\infty}^{\infty}\mathrm{sinc}^2\frac{\omega t}{2}\,d\omega = 1 - \frac{2\pi}{\hbar^2}W(0)t. \tag{6.10}$$

We see that in this range, the probability falls of linearly with time and that the decay rate is $2\pi/\hbar^2 \cdot W(0)$. Taking into account 6.8, those who are familiar with quantum mechanics should recognize this as the Fermi golden rule[5]. 6.10 also tells us why first order perturbation theory only applies when $t \ll \hbar^2/W(0)$: This

approximation scheme is best when the state of the system is close to the initial one. This means that the probability of still being in the initial state must be close to 1. We see from 6.10 that this will be the case only when $t \ll \hbar^2/W(0)$.

We now have three different expressions for the behavior of P at short times. 6.6 which applies when $t \ll \tau_2 = \hbar^2/W(0)$, 6.9 which applies when also $t \ll \tau_1 = \hbar/\Delta E$ and finally 6.10 which only applies when the timescale separation criterion $\tau_1 \ll \tau_2$ is satisfied, and then only in the range $\tau_1 \ll t \ll \tau_2$. These expressions should be compared numerically, but in order to do this we need a concrete expression for the function $W(\omega)$. We will operate in the continuum limit and define $W(\omega)$ as the maximally simple function

$$W(\omega) = \begin{cases} W & \text{for} \quad -\Delta\omega < \omega < \Delta\omega \\ 0 & \text{else} \end{cases}, \tag{6.11}$$

with W here being a constant.

With this definition, both 6.9 and 6.10 becomes very simple to calculate explicitly: 6.9 now simply becomes $P = 1 - 2W\Delta\omega t^2/\hbar^2$ while 6.10 becomes $1 - 2\pi W t/\hbar^2$. In order to also give a more explicit expression for 6.6 we first define the function $f(x)$ as

$$f(x) = \int_{-x}^{x} \operatorname{sinc} t \, dt = 2\int_{0}^{x} \operatorname{sinc} t \, dt. \tag{6.12}$$

Note that $f(x) \to \pi$ as $x \to \infty$. With this it is easily seen that in fact 6.6 becomes

$$P(t) = 1 - \frac{2t}{\hbar^2} W \cdot f\left(\frac{\Delta E t}{2\hbar}\right). \tag{6.13}$$

One can easily see from the expression itself that it has the correct behavior in the limits $t \ll \hbar/\Delta E$ and $t \gg \hbar/\Delta E$, but I shall also illustrate this with some plots (figure 6.1).

6.4 Redfield/Lindblad treatment

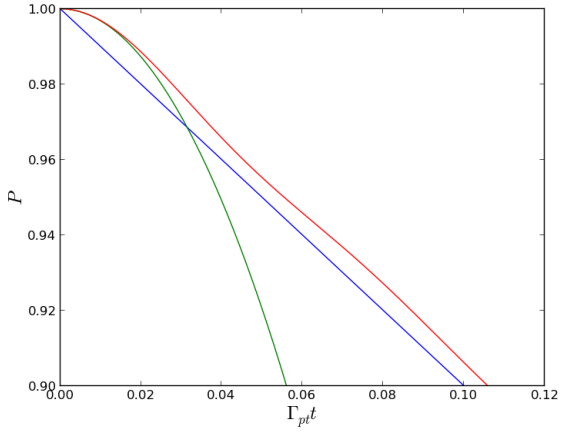
The treatment of the last section gave a pretty good picture of the short time behavior of the probability P for remaining in the excited state. At larger times however, first order perturbation theory fails and an other method is needed. In this section we will apply the Redfield equation 4.30, which we should remember applies only in the limit of weak interactions. This condition of weak interactions is really the same as the one which we in the last section called the time scale separation criterion: $\tau_1 \ll \tau_2$.

The first thing we should do when wishing to apply the Redfield equation to this model, is obviously to find the explicit form it takes in this case. However, due to similarity in form between the Hamiltonians of this model and the next, the derivations of the Redfield equations of these models will be completely identical and really only needs to be done once. Since in the next model we will also include effects of finite temperature, the derivation there will actually need to be more general. We will therefore delay the derivation to that chapter.

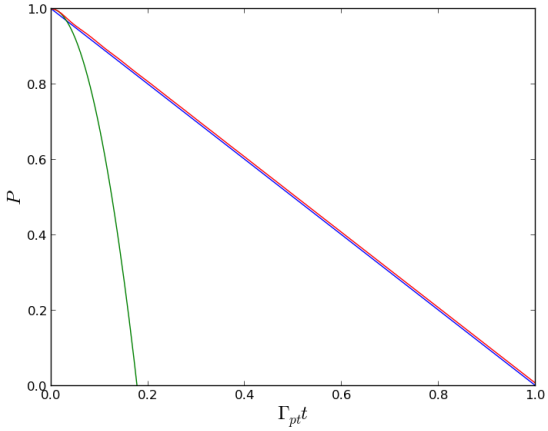
The final result when specializing to zero temperature can be found in 7.22, and is in Lindblad form. All we need to do to get the corresponding equation for the two-level model is to exchange the a and $a^\dagger$ operators with σ_- and σ_+. We then get

$$\dot{\rho} = -\frac{(E_0 + \delta)i}{\hbar}[P_e, \rho] + \Gamma(\sigma_- \rho \sigma_+ - \frac{1}{2}\{P_e, \rho\}), \tag{6.14}$$

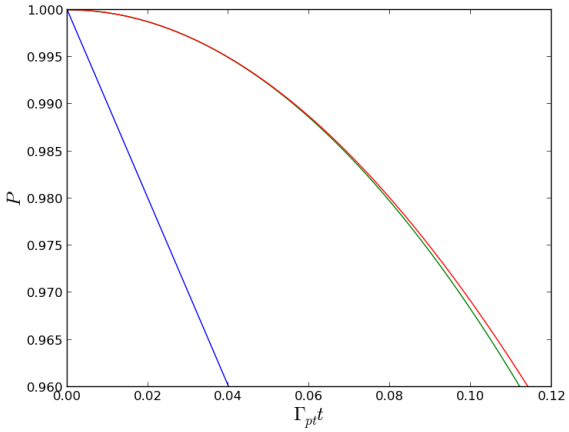
The expressions for Γ and δ may be found from the definitions below 7.18, and are found to be $\Gamma = 2\pi/\hbar^2 \cdot W(0)$ and $\delta = -\frac{1}{\hbar}\int \frac{d\omega}{\omega} W(\omega)$. The expression for Γ is identical to the Fermi golden rule expression, which makes sense since this parameter will be found to be the decay rate. The parameter δ is commonly denoted the 'Lamb shift', and it is something new relative to the previous treatment: Using perturbation theory, we would have needed to go to the second order to find this parameter.



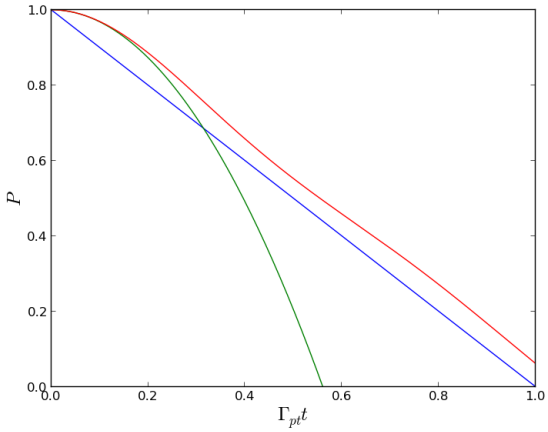
(a) $\Delta E = 100\hbar\Gamma_{pt}$, short time behavior.



(b) $\Delta E = 100\hbar\Gamma_{pt}$, long time behavior.



(c) $\Delta E = 10\hbar\Gamma_{pt}$, short time behavior.



(d) $\Delta E = 10\hbar\Gamma_{pt}$, long time behavior.

Figure 6.1: Comparison between the expressions $P = 1 - 2\pi Wt/\hbar$ (blue), $P = 1 - W\Delta Et^2/\hbar^2$ (green) and 6.13 (red). The quadratic curve always fits 6.13 at sufficiently short times. When $\Delta E = 100\hbar\Gamma_{pt}$ the linear curve lies quite close to 6.13 at all times, but for $\Delta E = 10\hbar\Gamma_{pt}$ it never lies really close to this, indicating that the timescale separation criterion fails for this small ΔE. Note also that all of the expressions eventually crosses zero, which means that none of them can be correct at large times.

Matrix expressions for P_e, σ_- and σ_+ can be found in section 2.3.1. Using these turns 6.14 into a four component matrix equation. However, since state operators are Hermitian and have trace 1, there are really only two independent equations:

$$\dot{P} = \dot{\rho}_{11} = -\frac{(E_0+\delta)i}{2\hbar}(\rho_{11}-\rho_{11}) + \Gamma(0-\frac{1}{2}(\rho_{11}+\rho_{11})) = -\Gamma P, \tag{6.15}$$

$$\dot{\rho}_{12} = -\frac{(E_0+\delta)i}{2\hbar}(\rho_{12}+\rho_{12}) + \Gamma(0-\frac{1}{2}(0+\rho_{12})) = -\left(\frac{(E_0+\delta)i}{\hbar}+\frac{1}{2}\Gamma\right)\rho_{12}, \tag{6.16}$$

These equations are easy to solve, and we get

$$P(t) = P(0)e^{-\Gamma t}, \tag{6.17}$$

$$\rho_{eg}(t) = \rho_{eg}(0)e^{-i(E_0+\delta)t/\hbar+\frac{1}{2}\Gamma t} \tag{6.18}$$

We see that we end up with an exponentially decaying excited state with decay rate Γ and energy shifted by δ. Assuming that $P(0) = 1$, we can find the short time behavior of 6.17 by making the linear expansion $P = e^{-\Gamma t} \approx 1 - \Gamma t$, which is in full agreement with 6.10. The expression is however linear also for very short times, and in particular it does not share the initially quadratic form of 6.9 and 6.6. So even though it may have the correct long time behavior, it does not behave correctly for very short times.

There is actually a very plausible explanation for this: The result is based on the Redfield equation 4.30. Upon deriving this equation we started out with 4.29 and argued that since the memory kernel is in any case very short, we might as well set the integration limit to infinity. However, this argument is not really valid when the time since initialization is shorter than the decay time of the memory kernel. To see whether this is indeed the problem, we will find and solve also 4.29.

To find this equation, it is easiest to start out with equation 7.13. This equation is derived from 4.30, so we must remember to replace the infinity sign in the time integral with t, as in 4.29. In addition to this we keep in mind that in the current case $T = 0$ so that also the number expectation $n(\beta, \Omega) = 0$. Also we once again replace a and $a^\dagger$ with σ_- and σ_+. It will also be usefull to define $\omega_0 = E_0/\hbar$. The result is

$$\begin{aligned}\dot{\rho} =& (2\sigma_-\rho\sigma_+ - \{P_e, \rho\})\frac{1}{\hbar^2}\int_0^t dt' \int d\omega W(\omega)\cos(\omega_0-\omega)t'/\hbar \\ &- [P_e, \rho]\frac{i}{\hbar^2}\int_0^t dt' \int d\omega W(\omega)\sin(\omega_0-\omega)t',\end{aligned} \tag{6.19}$$

which is still on Lindblad form. In fact, the only difference from 6.14 is that the parameters δ and Γ are now time dependent.

With this the equation for $P(t)$ becomes $\dot{P}(t) = -\Gamma(t)P(t)$, where $\Gamma(t)$ is given by

$$\begin{aligned}\Gamma(t) &= \frac{2}{\hbar^2}\int_0^t dt' \int d\omega W(\omega)\cos(\omega_0-\omega)t' \\ &= \frac{2}{\hbar^2}\int d\omega W(\omega)\frac{\sin(\omega_0-\omega)t}{\omega_0-\omega}.\end{aligned} \tag{6.20}$$

The solution to this equation (assuming $P(0) = 1$) is $P(t) = e^{-\int_0^t \Gamma(t')dt'}$. We calculate the integral in the exponent to be

$$\begin{aligned}\int_0^t \Gamma(t)dt &= \frac{2}{\hbar^2}\int_0^t dt' \int d\omega W(E)\frac{\sin(\omega_0-\omega)t'}{\omega_0-\omega} = \frac{2}{\hbar^2}\int d\omega W(\omega)\frac{1-\cos(\omega_0-\omega)t}{(\omega_0-\omega)^2} \\ &= \frac{4}{\hbar^2}\int d\omega W(\omega)\frac{\sin^2(\omega_0-\omega)t/2}{(\omega_0-\omega)^2} = \left(\frac{t}{\hbar}\right)^2\int d\omega W(\omega)\mathrm{sinc}^2\frac{(\omega_0-\omega)t}{2},\end{aligned} \tag{6.21}$$

and conclude that to the highest accuracy allowed by the Redfield weak interaction formalism we have

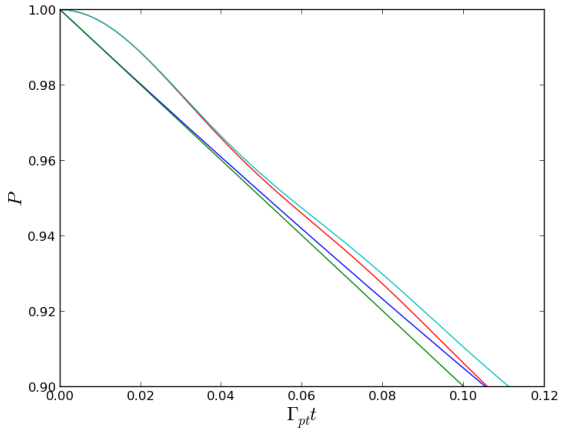
$$P(t) = \exp\left(-\left(\frac{t}{\hbar}\right)^2 \int d\omega W(\omega) \mathrm{sinc}^2 \frac{(\omega_0 - \omega)t}{2}\right), \tag{6.22}$$

an expression that should be compared to 6.6, which is obviously the 1. order expansion of 6.22.

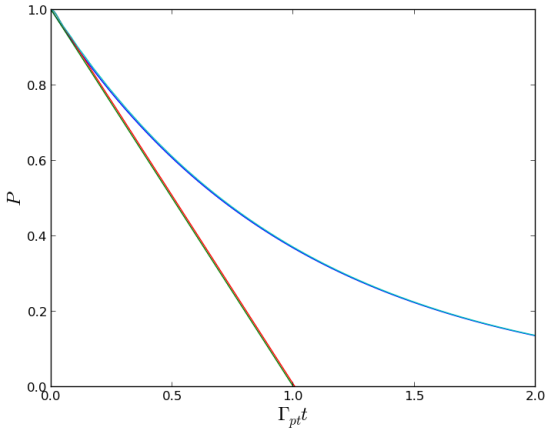
If we again assume the flat W function defined in 6.11, then clearly 6.22 becomes

$$P(t) = \exp\left(-\frac{2t}{\hbar} W \cdot f\left(\frac{\Delta E t}{2\hbar}\right)\right), \tag{6.23}$$

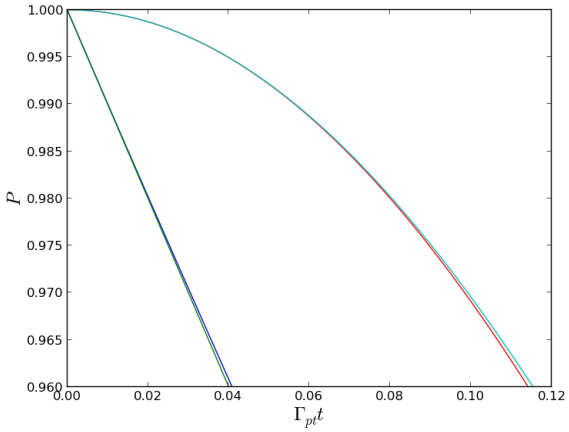
where $f(x)$ is still defined through 6.12 and we still have $\Delta E = \hbar\Delta\omega$. In figure 6.2 we compare 6.23 with 6.13, 6.10, as well as the simple formula $P = e^{-\Gamma t} = \exp(-2\pi W t/\hbar)$. We see that 6.23 has both the correct form at short times, ad the expected exponential form at large times. This could lead us to suspect that this is an exact expression. This is however not the case. Exact solutions we will first begin examining in the next section.



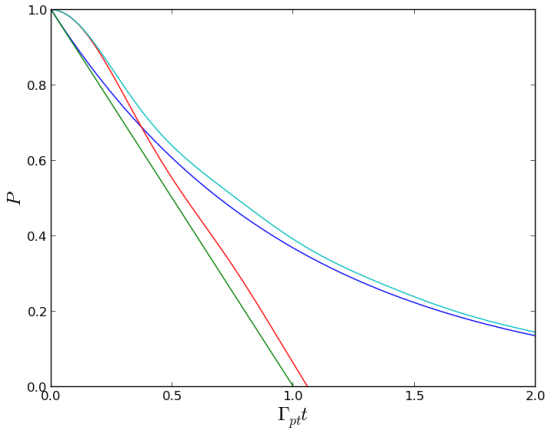
(a) $\Delta E = 100\hbar\Gamma_{pt}$, short time behavior.



(b) $\Delta E = 100\hbar\Gamma_{pt}$, long time behavior.



(c) $\Delta E = 10\hbar\Gamma_{pt}$, short time behavior.



(d) $\Delta E = 10\hbar\Gamma_{pt}$, long time behavior.

Figure 6.2: Comparison between the perturbation theory expressions $P = 1 - \Gamma t$ (green) and 6.13 (red), with the Redfield solutions $P = e^{-\Gamma t}$ (blue) and 6.23 (cyan). Note how at short times the exponential curve lies close to the linear one, while 6.23 lies close to 6.13. Note also that in the case of weak interactions (low Γ_{pt} compared to ΔE) 6.23 lies very close to the simple exponential curve.

6.5 Exact diagonalization

As mentioned in the beginning of the chapter, I limit the dynamics of our study to the subspace where states are on the form $c|e\rangle + c_g|g\rangle + \sum_k c_k|k\rangle$. Actually, the state $|g\rangle$ which does not interact with other states is only needed for expressing the results. For the purpose of solving the system this state can be ignored, so that the dimension of the remaining space is one more than the number of oscillators in the bath. If this number is not to large, the problem can be solved exactly using numerical diagonalization. That is to say, we let the Hamiltonian be represented by a matrix and then diagonalize the matrix numerically. We then express the state as a sum of eigenvectors, who's time development is simply $\Psi_k(t) = \Psi_k(0)e^{-iEt/\hbar}$. I have written a Python script that does this. The script calculates the coefficient $c(t)$ assuming that $c(0) = 1$. Let us call this quantity simply c. Knowing c makes it easy to find the reduced state, since $P(t) = P(0)|c|^2$ while $\rho_{12}(t) = \rho_{12}(0)c$.

As an example, according to the Lindblad type equation 6.14 we should have $c = e^{-i(E_0+\Delta E)t/\hbar + \frac{1}{2}\Gamma t}$. This however, is as we have seen only an approximation, and also it assumes a continuum of oscillators in the bath. To use exact diagonalization we must have a discrete and finite set of oscillators. But we can still make a quite good approximation to a continuum, so that given the right parameters the behavior should agree with 6.17 for some length of time.

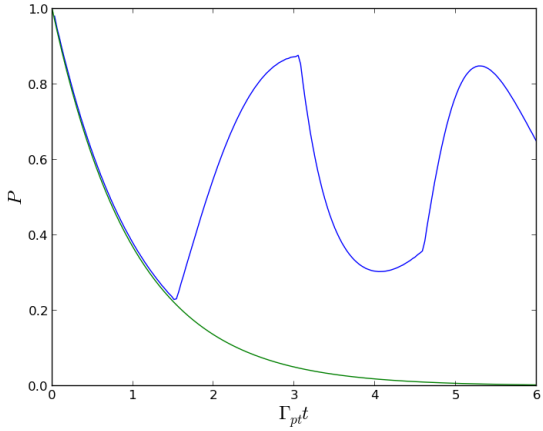
In order to do a numerical calculation, we need a concrete form of the interaction parameters w_k. We find this by making a discrete approximation to the continuous W function defined in 6.11: We let the bath consist of N oscillators with evenly spaced frequencies ω in the range from $\omega_0 - \Delta\omega$ to $\omega_0 + \Delta\omega$. The oscillators all have the same interaction strength $w_k = w = \sqrt{2W\Delta\omega/N}$ with the two-level system. The W function of this model becomes a better approximation to the continuous flat $W(\omega)$ when N becomes larger, or equivalently when the spacing $\delta\omega = 2\Delta\omega/(N-1)$ between the oscillators becomes smaller. We expect that for sufficiently small spacings the systems behavior will be like the continuous case for $t < T \sim 1/\delta\omega$. After this the phases of the oscillators will realign, creating interference effects.

To test this idea we will first compare the diagonalization results in the weak interaction limit ($W \ll \Delta E$) with the simple Redfield/Lindblad result 6.17. We see from figure 6.3 that our expectations are correct. The development agrees quite well with the exponential development of type 6.17 for times smaller than some critical value T at which there is a cusp in the graph. After this cusp the development changes its character completely. We also see from figure 6.3(a) and 6.3(d) that the cusps seem to repeat themselves periodically. The time T before the first cusp and the spacing between them seems to be the same, and this value increases more or less proportionally with N as expected. It is $1.53/\Gamma_{pt}$ for $N = 40$, $3.10/\Gamma_{pt}$ for $N = 80$ and $4.68/\Gamma_{pt}$ for $N = 120$. Here Γ_{pt} is the perturbation value for the decay rate (Fermi golden rule).

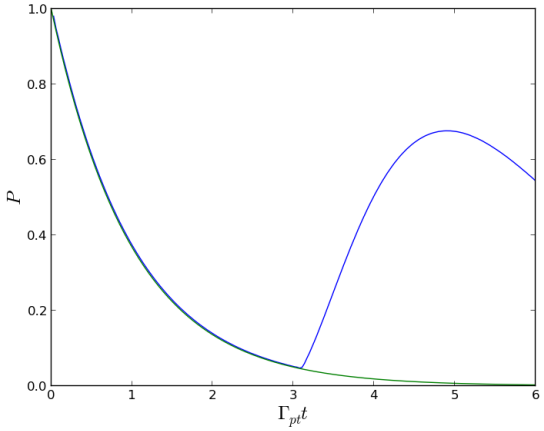
Assuming that $T = k/\delta\omega$ with k a dimensionless constant, we can try to find the value of this k. In the three cases above we find 6.28, 6.28 and 6.29 respectively. That is, all of them are approximately $2\pi \approx 6.28$, so it seems the formula $t_n = 2\pi n/\delta\omega$ will nicely describe the times t_n at which there are cusps. These are also precisely the times at which the oscillators, assuming that they start out with no phase difference, again have a phase difference of zero. We will examine the nature of these cusps in more detail in the next section.

6.3 thus indicates that solutions assuming a finite number of oscillators forms good approximations to the cases with continuous W functions in the range $t < 2\pi/\delta\omega$. We should now compare the diagonalization results also to our other approximations for these continuous cases, that is 6.22 and 6.6. This should illustrate how the exact development of the continuous case is when the time scale separation criterion is not satisfied. Actually, we already know how 6.22 and 6.6 relate to each other, and in particular we have found that 6.22 agrees both with 6.6 and the simple exponential result when these are supposed to be good.

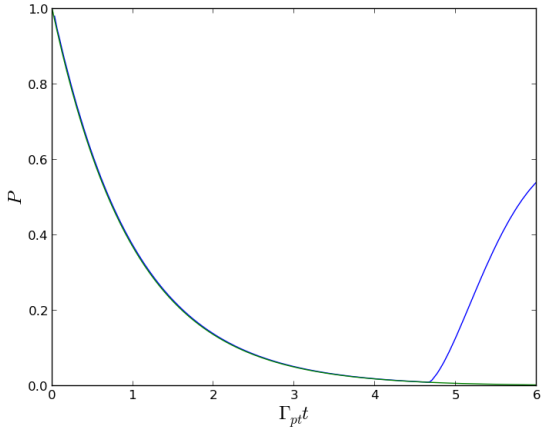
We will therefore only compare the exact diagonalization result with 6.22, or more precisely with 6.23 which 6.22 reduces to in the case of a flat W function. This is done in figure 6.4. The curves are in good agreement at short times or weak interactions. When the interactions are strong they are however not in agreement for large times. As mentioned we expect the diagonalization result to lie close to the



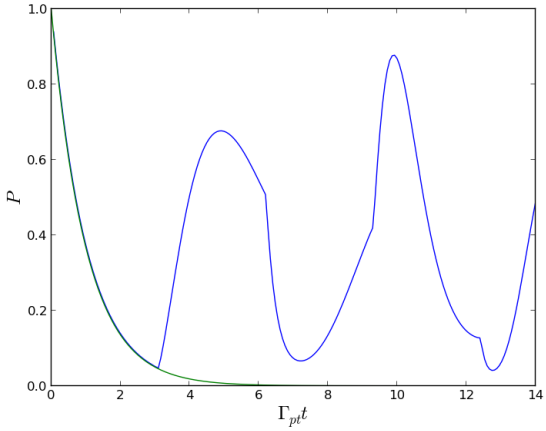
(a) $N = 40$, $\delta\omega = 4.103\Gamma_{pt}$. Cusps at $\Gamma_{pt}t = 1.53$, 3.05 and 4.59.



(b) $N = 80$, $\delta\omega = 2.025\Gamma_{pt}$. Cusp at $\Gamma_{pt}t = 3.11$.



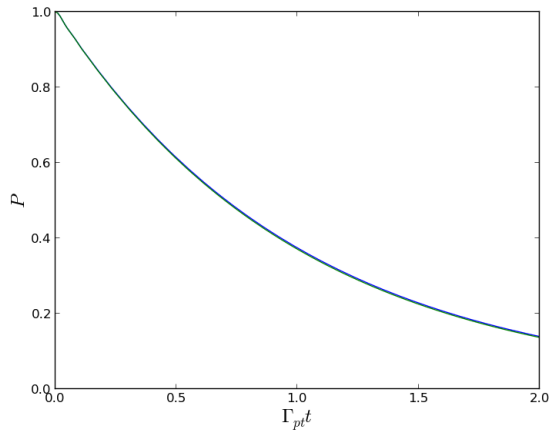
(c) $N = 120$, $\delta\omega = 1.345\Gamma_{pt}$. Cusp at $\Gamma_{pt}t = 4.68$.



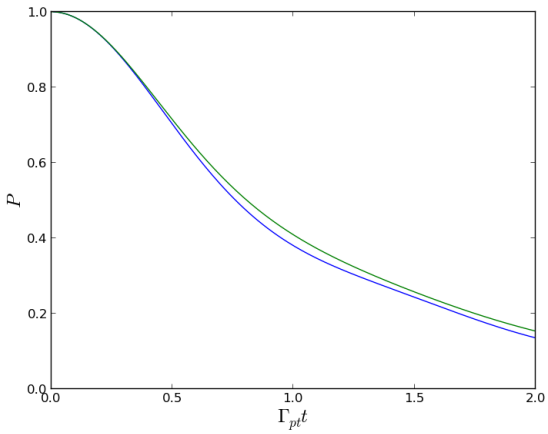
(d) $N = 80$, $\delta\omega = 2.025\Gamma_{pt}$. Long time behavior. Cusps at $\Gamma_{pt}t = 3.11$, 6.21, 9.30 and 12.39

Figure 6.3: Time development of probability for excited state in two-level system compared with simple exponential decay $P = e^{-\Gamma_{pt}t}$. It is assumed that $P(0) = 1$, so that $P = |c|^2$. Horizontal axis shows $\Gamma_{pt}t$, where $\Gamma_{pt} = 2\pi/\hbar \cdot W(0)$ is the decay rate according to the perturbation theory discussions. The calculation is done using the discrete model above, with a flat $W(\omega)$ function and $\Delta\omega = 80\Gamma_{pt}$. N, the number of oscillators is varied.

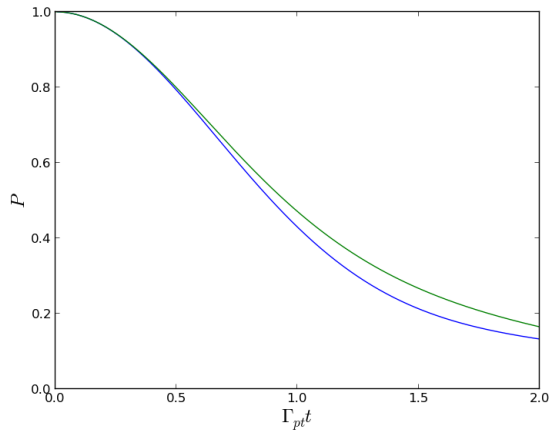
development in the continuum limit. We thus interpret this as demonstrating that 6.22 is not an exact solution.



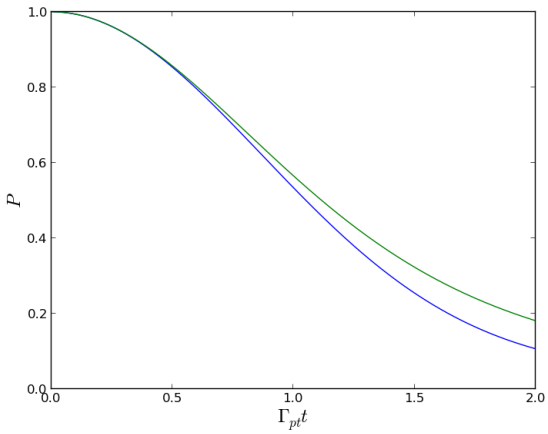
(a) $\Delta E = 100\hbar\Gamma_{pt}$.



(b) $\Delta E = 5\hbar\Gamma_{pt}$r.



(c) $\Delta E = 3\hbar\Gamma_{pt}$.

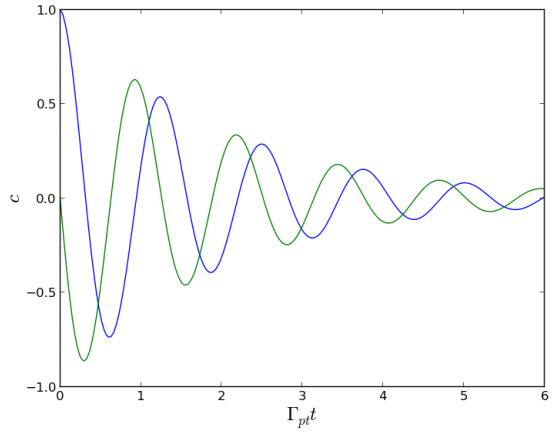


(d) $\Delta E = 2\hbar\Gamma_{pt}$.

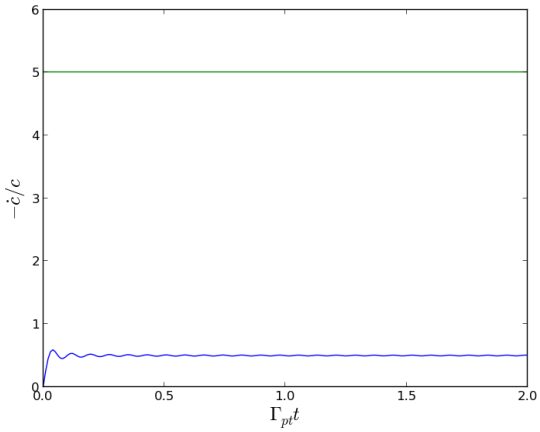
Figure 6.4: Comparison between the Redfield solution 6.23 (green) and the exact diagonalization result (blue). Unsurprisingly, when the timescale separation criterion holds the curves are almost inseparable. When the time scale separation is violated the curves agree at sufficiently short times, but disagree at large ones. The disagreement increases with stronger interactions. In this model, the exact solution is damped faster than the Redfield approximation.

Up til now all our analysis has been of the probability $P = |c|^2$. The last subject of this section will therefore be the behavior of c it self. The development of c is shown in figure 6.5. In 6.5(a) we can see the cyclic behavior of $c(t)$, which gives us information about the energy of the system. In 6.5(b) I have plotted the quantity $-\dot{c}/c$, which according to the simple Lindblad solution should be $\Gamma/2 + i(E_0 + \delta)/\hbar$. In 6.5(c) the deviations of the real part of this quantity from $\Gamma/2$ is shown. As all ready known, these show us that the decay is not exactly exponential. Finally, in 6.5(d) I have plotted the deviations of the imaginary part from $E_0/\hbar$. This should correspond to the Lamb shift δ. As we see, this is of the order 10^{-14} and so, within numerical error essentially 0.

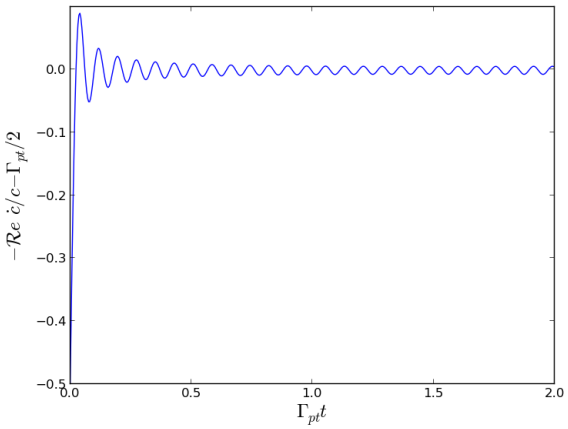
We should compare this numerical result for the Lamb shift with the expression $\delta = -\int \frac{d\omega}{\omega} W(\omega)$ found during the Redfield analysis. With our flat W function this becomes $\delta = -W \int_{-\Delta\omega}^{\Delta\omega} \frac{d\omega}{\omega}$. Since the integrand is antisymmetric, the integral is 0 just like the numerical result. However, if we had a slightly different W function, we could get something different from 0. The simplest choice is to keep $W(\omega) = 0$ outside of the range $[\omega_0 - \Delta\omega, \omega_0 + \Delta\omega]$, but change it to the linear function $W(\omega) = (1 + p(\omega - \omega_0)/\Delta\omega)W$



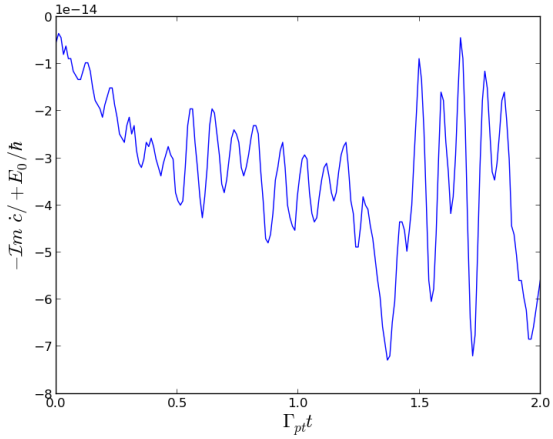
(a) c



(b) $-\dot{c}/c$



(c) $-\mathcal{R}e\,\dot{c}/c - \Gamma_{pt}/2$



(d) $-\mathcal{I}m\,\dot{c}/c + E_0/\hbar$

Figure 6.5: The behavior of $c(t)$. Calculation is done with $E = 5\hbar\Gamma_{pt}$, $\Delta\omega = 80$ and $N = 160$. The two upper plots show the imaginary and real parts of c it self and of $-\dot{c}/c$. The lower plots show $-\mathcal{R}e\,\dot{c}/c-\Gamma_{pt}/2$ and $-\mathcal{I}m\,\dot{c}/c - E/\hbar$, which corresponds to the deviation from the perturbation decay rate and the Lamb shift respectively.

inside it. The integral then changes to

$$\delta = -W \int_{-\Delta\omega}^{\Delta\omega} \frac{1 + p\omega/\Delta\omega}{\omega} d\omega = -2pW = -\frac{p\hbar\Gamma_{pt}}{\pi}. \tag{6.24}$$

In figure 6.6 $-\mathcal{I}m\,\dot{c}/c - E/\hbar$ is shown again, but now with the linear W function with different values of p. In all cases we get a value that oscillates with a small amplitude around an average. For $p = 0.1$, 0.5 and 0.8 this average is -0.032$\hbar\Gamma_{pt}$, -0.16$\hbar\Gamma_{pt}$ and -0.26$\hbar\Gamma_{pt}$ respectively. On the other hand, using the formula 6.24 we get -0.032$\hbar\Gamma_{pt}$, -0.16$\hbar\Gamma_{pt}$ and -0.25$\hbar\Gamma_{pt}$. This is close enough to conclude that we again have agreement between the perturbation expression and the numerical results.

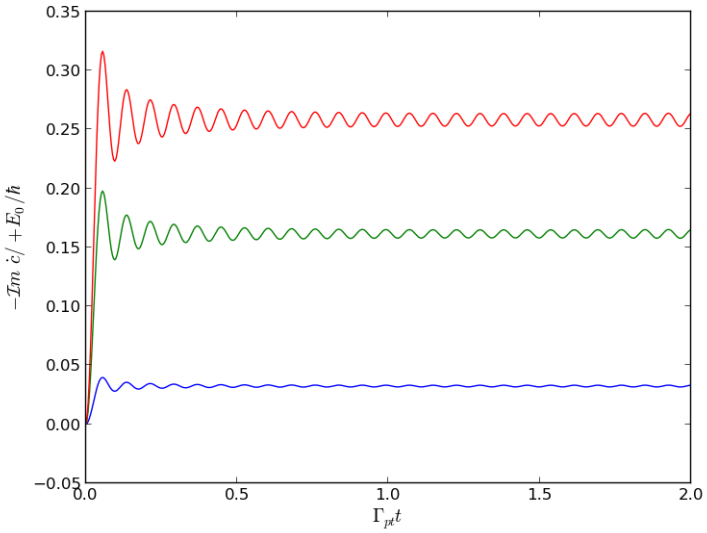


Figure 6.6: $-\mathcal{I}m\,\dot{c}/c - E/\hbar$ with $W(E) = (1 + p(E - E_0)/\Delta E)W$ in the range $[E_0 - \Delta E, E_0 + \Delta E]$. The calculation is done with $E = 5\hbar\Gamma_{pt}$, $\Delta\omega = 80$ and $N = 160$. The blue curve corresponds to $p = 0.1$, the green one to $p = 0.5$ and the red to $p = 0.8$. These curves oscillate around the averages -0.032$\hbar\Gamma_{pt}$, -0.16$\hbar\Gamma_{pt}$ and -0.26$\hbar\Gamma_{pt}$ respectively.

6.6 Exact memory kernel

The exact diagonalization results obtained in the previous section are obviously only truly exact when we are dealing with a discrete and finite number of oscillators, and the W function accordingly is a finite sum of delta functions. When the W function is continuous, as it is in the cases treated in the perturbation an Redfield formalisms, these results are only approximations believed to increase in accuracy when $\delta\omega$ decreases. It would therefore be nice if we also had some other exact method that we could compare the results to.

One of the reasons we look at precisely this model is that there actually exists such a method. It turns out that the system can be described by a memory equation of type 5.16 where the memory kernel $\mathcal{K}(t, t')$ is exactly calculable. This will allow us to apply any method that can be used to solve such equations. Due to the Nakajima Zwanzieg formalism these are in any case highly relevant to the treatment of open systems, which is another reason to have a look at this particular description.

The existence of this scalar memory equation was something I originally discovered myself as I worked with this model, and the entire analysis of this section is really my own invention. Later I have however discovered (unsurprisingly I must admit) that this method has already been employed elsewhere: It is derived also in [2], and according to them the method was originally employed By Wigner and Weisskopf in [14].

Unlike the Nakajima Zwanzieg equation the memory equation to be treated here is not expressed in terms of the reduced state operator ρ_S, but instead in terms of the probability amplitude $c(t)$ for S being in its excited state $|e\rangle$. Because of the simplicity of the system, knowing this and the initial state is enough to completely specify $\rho_S(t)$ at any time by the simple formula

$$\rho_S(t) = \begin{pmatrix} |c(t)|^2 P(0) & c(t)\rho_{12}(0) \\ c^\star(t)\rho_{21}(0) & 1 - |c(t)|^2 P(0) \end{pmatrix}. \tag{6.25}$$

The Nakajima Zwanzieg equation of this system will be treated in the next section.

6.6.1 Derivation

We begin by again making the expansion $|\psi\rangle = c(t)\,|e\rangle + \sum_k c_k(t)\,|k\rangle$. In the interaction picture this state will evolve according to the equation $\hbar i|\dot{\psi}\rangle = H_{SE}(t)\,|\psi\rangle$, where $H_{SE}(t) = e^{iH_0 t/\hbar} H_{SE}(0) e^{-iH_0 t/\hbar}$ and $H_{SE}(0)$ is the Schrodinger picture operator. Inserting the expansion of $|\psi\rangle$ in to this, as well as 6.2, we get the following equations for c and the c_ks:

$$i\hbar\dot{c} = \sum_k w_k e^{-i\omega_k t + iEt/\hbar} c_k, \tag{6.26}$$

$$i\hbar\dot{c}_k = w_k^\star e^{i\omega_k t - iEt/\hbar} c. \tag{6.27}$$

We then define the function $f(\omega, t)$ as

$$f(\omega, t) = \sum_k w_k c_k(t) \delta(\omega - \omega_k + E_0/\hbar), \tag{6.28}$$

which makes us able to rewrite the equations 6.26 as

$$\frac{dc}{dt}(t) = \frac{1}{\hbar i} \int_{-\infty}^{\infty} f(\omega, t) e^{-i\omega t} d\omega, \tag{6.29}$$

$$\frac{\partial f}{\partial t}(\omega, t) = \frac{1}{\hbar i} W(\omega) e^{i\omega t} c, \tag{6.30}$$

where $W(\omega)$ is the function defined in 6.7. These equations show that $W(\omega)$ is in fact the only information we need of the environment in order to determine the exact development of $c(t)$. Note that we could now choose to take the continuum limit, which would make $f(\omega, t)$ and $W(\omega)$ continuous functions of ω. Nothing in the following derivation will be different whether this is done or not.

The next thing we do is to construct a new function g as the Fourier transform of f:

$$g(x, t) = \int_{-\infty}^{\infty} f(\omega, t) e^{-i\omega x} d\omega. \tag{6.31}$$

we can once again rewrite the equations describing the system in terms of this function. 6.29 now gives us

$$\frac{dc}{dt}(t) = \frac{1}{\hbar i} g(t, t), \tag{6.32}$$

$$\frac{dg}{dt}(x, t) = \int_{-\infty}^{\infty} \frac{df}{dt}(\omega, t) e^{-i\omega x} d\omega = \frac{1}{\hbar i} \int_{-\infty}^{\infty} W(\omega) e^{i\omega t - i\omega x} c(t)\, d\omega = \hbar i K(x - t) c(t), \tag{6.33}$$

where we have also made the definition

$$K(t) = -\frac{1}{\hbar^2} \int_{-\infty}^{\infty} W(\omega) e^{-i\omega t} d\omega, \tag{6.34}$$

which is in fact the memory kernel. Or more precisely the memory kernel is $K(t-t')$. Starting out with 6.32 this is easily demonstrated: At $t=0$ the environment is in the vacuum state, so the c_ks are all zero. From the definitions we therefore also have $f(\omega,0)=g(x,0)=0$. We can then integrate 6.33 to get

$$g(x,t)=\int_0^t \frac{dg}{dt}(x,t')dt'=\hbar i\int_0^t K(x-t')c(t')dt', \tag{6.35}$$

which can then be inserted into 6.32. This finally gives

$$\frac{dc}{dt}(t)=\int_0^t K(t-t')c(t')dt'=\int_0^t K(t')c(t-t')dt', \tag{6.36}$$

which is an exact integro differential equation for the probability amplitude $c(t)$, involving the memory kernel $K(t)$.

6.6.2 Markovian limit

The equation 6.36 has a memory kernel $K(t)$ that can be calculated exactly. This can be used to see very directly where the timescale separation criterion discussed earlier actually comes from. Let us assume that $K(t)$ is effectively damped out over some characteristic time scale τ, in the sense that most of the last integral in 6.36 comes from the region $0<t'<\tau$. Let us further assume that τ is very small compared to the timescale over which $c(t)$ changes. It then becomes justified to approximate the equation as

$$\frac{dc}{dt}(t)\approx\int_0^\infty K(t')c(t)dt'=-\gamma c(t), \tag{6.37}$$

with $\gamma=-\int_0^\infty K(t)dt$. This could also be thought of as replacing the memory kernel with $K(t)=-\gamma\delta(t)$. Such a delta function memory could be said to be the defining property of Markovian development.

6.37 has the exponential solution $c(t)=e^{-\gamma t}$, which is identical to the result obtained through the Redfield formalism (Whether the quantity γ has the correct value will be discussed below). In fact the Redfield/Lindblad equation 6.14 can itself also be derived by combining 6.37 with 6.25.

I mentioned earlier that 6.14 applies in the cases where we have time scale separation. We are now in a position to demonstrate this: As mentioned 6.37 applies when $K(t)$ is short, in the sense that its damping timescale τ is much smaller than the scale over which c changes, which is essentially $|c/\dot{c}|$. Let us construct some estimates for these time scales: $\dot{c}$ is given by 6.36, so as a quite reasonable estimate of the quantity $|\dot{c}/c|$ we could take the integral $\int_0^\infty K(t')dt'$, or alternatively $\frac{1}{2}\int_{-\infty}^\infty K(t')dt'$. We will use the later, since by applying the inverse Fourier transform to 6.34 we see that this can be written simply as $-\pi W(0)/\hbar$. Thus we conclude that $|c/\dot{c}|\sim\hbar/W(0)$, which we recognize as the definition of τ_2.

In order to get an estimate of the quantity τ, we need a more precise definition of this: Since τ is the length of the interval in which $K(t)$ is significantly different from 0, the integral $\int_{-\infty}^\infty K(t)dt$ will be of order $2K(0)\tau$. So one possible definition is to simply let τ be given by the expression $K(0)\tau=\frac{1}{2}\int_{-\infty}^\infty K(t)dt$. Again applying the Fourier Transform and its inverse together with 6.34 to this expression, we see that it can be re-expressed as $2\tau\int_{-\infty}^\infty W(\omega)d\omega=2\pi W(0)$. Now defining $\Delta\omega$ in much the same way through the relation $W(0)\Delta\omega=\frac{1}{2}\int_{-\infty}^\infty W(\omega)d\omega$, we see that in fact $\tau=\pi/2\Delta\omega\approx\hbar/\Delta E$. This we recognize as the definition of τ_1. Thus clearly the condition for Markovianness can be written simply as $\tau_1\ll\tau_2$, which is the aforementioned timescale separation criterion.

Let us now attempt to find the value of γ, in order to verify that the expression agrees with our earlier results. Let $u(t)$ be the unit step function. Then

$$\begin{aligned}\gamma=&-\int_{-\infty}^\infty K(t)u(t)dt=\frac{1}{\hbar^2}\int_{-\infty}^\infty u(t)\int_{-\infty}^\infty W(\omega)e^{-i\omega t}d\omega dt=\frac{1}{\hbar^2}\int_{-\infty}^\infty W(\omega)\int_{-\infty}^\infty u(t)e^{-i\omega t}dtd\omega\\ =&\frac{1}{\hbar^2}\int_{-\infty}^\infty W(\omega)\left(\frac{1}{i\omega}+\pi\delta(\omega)\right)d\omega=\frac{\pi}{\hbar^2}W(0)-\frac{i}{\hbar^2}\int_{-\infty}^\infty\frac{W(\omega)}{\omega}d\omega,\end{aligned} \tag{6.38}$$

in complete agreement with both the perturbation result and the Redfield equation.

6.6.3 Asymptotic exponential solutions

In many cases, the equation 6.36 admits an approximate exponential solution even when a Markovian approximation like this is not defendable. As long as the memory kernel falls of over some time scale, however large, then for sufficiently large t the equation can be approximated as

$$\frac{dc}{dt}(t) = \int_0^\infty K(t')c(t-t')dt', \tag{6.39}$$

which under appropriate conditions has an exact exponential solution: Inserting the ansatz $c(t) = e^{-\gamma t}$ into it, we end up with the integral equation

$$-\gamma = \int_0^\infty K(t)e^{\gamma t}dt. \tag{6.40}$$

If some γ is a solution to this equation, then $c(t) = e^{-\gamma t}$ will be a solution of 6.39. Note that it is a solution for all t, not only $t > 0$.

Now, 6.40 is expressed in terms of the memory kernel $K(t)$. We can also get an equation for γ directly in terms of the W function: We do this by going back to the equations 6.29 and 6.30, and again insert the ansatz $c(t) = e^{-\gamma t}$. With this ansatz 6.30 becomes $\dot{f} = -iW(\hbar\omega)e^{i\omega t-\gamma t}$, which has the solution

$$f(\omega, t) = \frac{W(\omega)e^{i\omega t-\gamma t} + h(\omega)}{\hbar i(i\omega - \gamma)}, \tag{6.41}$$

with $h(\omega)$ being some freely chosen function. We then insert this in 6.29 to get

$$\gamma e^{-\gamma t} = \frac{1}{\hbar^2}\int_{-\infty}^\infty \frac{W(\omega)e^{-\gamma t} + h(\omega)e^{-i\omega t}}{i\omega - \gamma}d\omega. \tag{6.42}$$

Since there are no functions that have Fourier transforms which are proportional to $e^{-\gamma t}$ for all t, the only way this equation can be satisfied for all t is if $h(\omega) = 0$. This turns 6.42 into

$$\gamma = \frac{1}{\hbar^2}\int_{-\infty}^\infty \frac{W(\omega)}{i\omega - \gamma}d\omega, \tag{6.43}$$

the sought integral equation in terms of W.

Note that exponential solutions found using either 6.40 or 6.43 are nonphysical: They both assume the solutions to have the same exponential form also for $t < 0$, which means that the probability $P = |c|^2$ will be bigger than 1 for these times. However, since 6.39 as mentioned is the asymptotic limit of the exact memory equation of the system, it is reasonable to assume that the solutions to this equation may form the asymptotic evolution of $c(t)$. This would then also lead us to expect that the γ that solves 6.40 will be a better value for this parameter than the one found using the simple Markovian limit.

But what about 6.43? Is this an equivalent condition? Well, 6.43 expresses all the possible exponential solutions to 6.29 and 6.30, and the solutions to 6.40 must obviously be contained in this set. But in principle it is possible that 6.43 has additional solutions. We will quickly see that examples of such solutions are easy to find. These, not solving 6.39, will not form asymptotic solutions to 6.36. Unlike the solutions to 6.40 we can therefore not expect these to be asymptotic evolutions of $c(t)$.

In order for 6.40 to have a solution the involved integral must be defined, and so $K(t)$ must fall off at least exponentially. The flat W defined by 6.11 gives an example of a system where this is not the case. This is because this W function will give rise to a memory kernel proportional to $\operatorname{sinc}\Delta\omega t$, which falls of as $1/t$ and thus slower than exponentially. Even so we can still find solutions to 6.43, which then becomes

$$\gamma = \frac{W}{\hbar^2}\int_{-\Delta\omega}^{\Delta\omega}\frac{1}{i\omega - \gamma}d\omega = -\frac{W}{\hbar^2}\int_{-\Delta\omega}^{\Delta\omega}\frac{i\omega + \gamma}{\omega^2 + \gamma^2}d\omega = \frac{2W}{\hbar^2}\arctan\frac{\Delta\omega}{\gamma}, \tag{6.44}$$

and always have at least one solution. This simple flat W function is thus an example demonstrating that 6.40 and 6.43 are not equivalent.

I will give one more such example: $W(\omega) = We^{-|\omega|/\Delta\omega}$. This will cause $K(t)$ to be a Lorenzian function, falling of as $1/t^2$ for large t, and thus again slower than exponentially. Still, 6.43 ends up as

$$\gamma = -\frac{2W}{\hbar^2}\int_0^\infty \frac{\gamma e^{-\omega/\Delta\omega}}{\omega^2+\gamma^2}d\omega. \tag{6.45}$$

Just as in the case of any other W function, the expression to the right must start out at the perturbation/Redfield expression $\pi W/\hbar^2$ when $\gamma \to 0$. A way to see this directly from the expression is to change the variable of integration to $x = \omega/\gamma$. Also, when $\gamma \to \infty$ it goes to 0. It therefore clearly must cross the line described by the left expression, and thus the equation must again have at least one solution.

Having now dealt with a case where 6.40 does not have a solution, we should turn to one where it has. The simplest case, where we even have a purely algebraic solution, is to let $W(\omega)$ be a Lorenzian function: $W(\omega) = \frac{W\Delta\omega^2}{\omega^2+\Delta\omega^2}$. This would give us the exponential memory kernel $K(t) = -\frac{\pi W\Delta\omega}{\hbar^2}e^{-\Delta\omega t}$ for $t > 0$. Inserting this into 6.40 we get the simple second order equation

$$\gamma = \frac{\pi W\Delta\omega}{\hbar^2}\frac{1}{\Delta\omega-\gamma}, \tag{6.46}$$

as long as $\gamma < \Delta\omega$. If this is not the case, the integral does not converge. The solutions are

$$\gamma = \frac{\Delta\omega}{2}\left(1 \pm \sqrt{1-\frac{4\pi W}{\hbar^2\Delta\omega}}\right), \tag{6.47}$$

which both are smaller than $\Delta\omega$ and thus valid. It is however only the one with the minus sign that is close to the perturbation value for small W, so we expect this to give the correct asymptotic evolution. For $\Delta\omega > 2\Gamma_{pt}$ we now have

$$\Gamma = \Delta\omega\left(1 - \sqrt{1-\frac{2\Gamma_{pt}}{\Delta\omega}}\right), \tag{6.48}$$

which is easily seen to have the limit $\Gamma = \Gamma_{pt}$ when $\Delta\omega \to \infty$. Here Γ is the exact asymptotic decay rate of $P(t)$ given by $\Gamma = 2\mathcal{R}e\,\gamma$, while Γ_{pt} is as before the perturbation/Redfield expression for this parameter.

I also include another W function which causes $K(t)$ to fall off sufficiently fast, namely $W(\omega) = We^{-\frac{\omega^2}{2\Delta\omega^2}}$. This makes $K(t) \sim e^{-\frac{\Delta\omega^2}{2}t^2}$. Here I omit the details, but in the end we end up with the equation

$$\frac{\Gamma}{\Gamma_{pt}} = e^{\frac{\Gamma^2}{8\Delta\omega^2}}\left(1 + \mathrm{erf}\left(\frac{\Gamma}{\sqrt{8}\Delta\omega}\right)\right), \tag{6.49}$$

where the erf function is $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$. This equation can not be solved analytically, but numerically it is no problem. Both this and 6.48 will later be compared with actual rates from simulations.

6.6.4 Discrete W-function

The memory equation 6.36 is not only a power full tool for analyzing exponential evolution, but also departures from this. Remember for instance our discussion of figure 6.3, where the development keeps its exponential character for a characteristic time $T = 2\pi/\delta\omega$ and then rapidly takes on a completely different behavior. By help from the exact memory kernel it becomes possible to see why making a discrete approximation to the W function causes this type of behavior: Assume that we replace some general W function with the discrete approximation

$$W_d(\omega) = W(\omega)\delta\omega\sum_{n=-\infty}^{\infty}\delta(\omega - n\delta\omega - f\delta\omega), \tag{6.50}$$

where the quantity f is some number $0 \leq f < 1$ that describes the translational shift of the sequence of delta functions.

What is the relation ship between the memory kernel of this approximation and that of $W(\omega)$? Let K_d be the memory kernel corresponding to W_d. From 6.34 we see that

$$K_d(t) = -e^{-if\delta\omega t}\frac{1}{\hbar^2}\sum_{n=-\infty}^{\infty}\delta\omega W(n\delta\omega)e^{-in\delta\omega t}. \tag{6.51}$$

The phase factor $e^{-if\delta\omega t}$ complicates things, so let us first analyze the function $K_d(t)e^{if\delta\omega t}$. We first note that this is periodic with period $2\pi/\delta\omega$. Secondly we note that it has the form of a Fourier series with coefficients $C_n = -\delta\omega W(n\delta\omega)/\hbar^2$. Now once more applying the inverse Fourier transform to 6.34 we see that these coefficients can be written

$$C_n = -\frac{1}{\hbar^2}\delta\omega W(n\delta\omega) = \frac{\delta\omega}{2\pi}\int_{-\infty}^{\infty}K(t)e^{in\delta\omega t}dt. \tag{6.52}$$

Let us now assume that we have made the discrete approximation sufficiently dense ($\delta\omega$ sufficiently small) to assure that the damping time $\tau = \tau_1$ of $K(t)$ is considerably shorter than $\pi/\delta\omega$. We are then free to approximate the integral above to get

$$C_n = \frac{\delta\omega}{2\pi}\int_{-\infty}^{\infty}K(t)e^{in\delta\omega t}dt \approx \frac{\delta\omega}{2\pi}\int_{-\pi/\delta\omega}^{\pi/\delta\omega}K(t)e^{in\delta\omega t}dt, \tag{6.53}$$

which should be recognized as precisely the Fourier coefficients of the function $K(t)$ when limited to the range $[-\pi/\delta\omega, \pi/\delta\omega]$. From this we conclude that for sufficiently dense oscillator sets ($\delta\omega \ll \Delta\omega$), the function $e^{if\delta\omega t}K_d(t) = K(t)$ in the range $[-\pi/\delta\omega, \pi/\delta\omega]$. Since the function has period $2\pi/\delta\omega$, the values in this range is also repeated periodically outside it. That is, we essentially have

$$K_d(t) \approx e^{-if\delta\omega t}\sum_{n=-\infty}^{\infty}K(t - 2\pi n/\delta\omega), \tag{6.54}$$

where the fact that $K(t)$ is practically 0 outside of the range $[-\pi/\delta\omega, \pi/\delta\omega]$ has again been used.

If K also falls of sufficiently fast to satisfy the time scale separation criterion $\tau_1 \ll \tau_2$ as discussed above, then K_d can be approximated further as a sum of delta functions. When doing this it is important to keep in mind that the domain of integration in 6.36 extends only from 0 to t. This first of all means that we do not need to include the the terms in 6.54 where $n < 0$. Secondly, and more importantly, it has consequences for the coefficients that should be put in front of the delta functions:

For terms with $n > 0$ the integral will extend over the entire region where the term is large, so that the coefficients should in these cases be $\Gamma = -\int_{-\infty}^{\infty}K(t)dt = 2\mathcal{R}e\gamma$. For the $n = 0$ term however, the integral only extends over half the term, so that the coefficient should be $\gamma = -\int_{0}^{\infty}K(t)dt$. Because of this we should take K_d to be

$$K_d(t) = -\gamma\delta(t) - e^{-if\delta\omega t}\Gamma\sum_{n=1}^{\infty}\delta(t - 2\pi n/\delta\omega)), \tag{6.55}$$

which makes 6.36

$$\dot{c}(t) = -\gamma c(t) - \Gamma\sum_{n=1}^{m}e^{-i2\pi fn}c(t - 2\pi n/\delta\omega)), \tag{6.56}$$

with m being the largest integer such that $t - 2\pi m/\delta\omega > 0$. We can see directly from this equation that the behavior of $c(t)$ will change abruptly whenever t crosses an integer multiple of $2\pi/\delta\omega$: This will make m increase by 1, so that the equation gets an additional term and thus completely changes nature. This

gives us an explanation of the periodic cusps that was seen for instance in figure 6.3. In fact we will now attempt to use 6.56 to provide a complete reconstruction of the development in figure 6.3(d):

In the calculation which resulted in that figure, the oscillators were distributed evenly in the range $[-\Delta\omega, \Delta\omega]$ and thereby symmetrically around 0. This means that the shift f must be either 0 or $\frac{1}{2}$. It will be 0 when the number of oscillators is odd, and $\frac{1}{2}$ when it is even. In 6.3(d) 80 oscillators was used, so that $f = \frac{1}{2}$ and in particular $e^{-i2\pi fn} = (-1)^n$. With this all parameters involved in 6.56 are well defined, and we can proceed with the solution. For simplicity we will use units where $\Gamma = \Gamma_{pt} = 1$ and define $T = 2\pi/\delta\omega$. We also keep in mind that the W function is on the form 6.11, so that the Lamb shift $\delta = 0$ and γ is just $\gamma = \Gamma/2 = 1/2$.

As mentioned the behavior of $c(t)$ will depend on what range t is in. We therefore define the functions $u_n(t)$ such that $c(t) = u_n(t)$ in the range $[nT, (n+1)T]$. Imposing 6.56 and the definitions above, the functions $u_n(t)$ must then clearly satisfy

$$\dot{u}_n(t) = -\frac{1}{2}u_n(t) - \sum_{k=1}^{n}(-1)^k u_{n-k}(t - kT). \tag{6.57}$$

We then further define $u_n(t) = f_n(t - nT)e^{-\frac{1}{2}(t-nT)}$, which makes the functions f_n satisfy the equations

$$\dot{f}_n(t) = -\sum_{k=0}^{n-1}(-1)^{n-k} f_k(t). \tag{6.58}$$

In addition, the continuity of $c(t)$ means $u_n(nT) = u_{n-1}(nT)$, and thus $f_n(0) = f_{n-1}(T)e^{-\frac{1}{2}T}$. This makes the solution to 6.58 simply

$$f_n(t) = f_{n-1}(T)e^{-\frac{1}{2}T} - \sum_{k=0}^{n-1}(-1)^{n-k}\int_0^t f_k(t')\,dt', \tag{6.59}$$

for $n > 0$. We see immediately that $f_0(t) = 1$. Now defining $K = e^{-\frac{1}{2}T}$, we add together the above equation with the corresponding for $f_{n-1}(t)$. Since $(-1)^{(n-1)-k} = -(-1)^{n-k}$, all terms in the sum except for one will cancel, so that we end up with the relatively simple recursive formula

$$f_n(t) = f_{n-1}(0) - f_{n-1}(t) + f_{n-1}(T)K + \int_0^t f_{n-1}(t')\,dt'. \tag{6.60}$$

From this we find

$$\begin{aligned} f_1(t) =& K + t, \\ f_2(t) =& -t + (K+T)K + Kt + \frac{1}{2}t^2, \\ f_3(t) =& t - Kt - t^2 - Kt + K^3 + 2K^2T + \frac{1}{2}KT^2 + \frac{1}{6}t^3 + \frac{1}{2}t^2K + K^2t + KTt. \end{aligned} \tag{6.61}$$

For the purpose of comparison with the numerics I have also found the expression for f_4. It is however somewhat long, ugly, and uninformative, so I do not include it in the text.

With the expressions for the f_ns now found, we can use $c(t) = u_n(t) = f_n(t - nT)e^{-\frac{1}{2}(t-nT)}$ for $t \in [nT, (n+1)T]$ to calculate the evolution of the probability $P = |c|^2$ and compare this with the numerical results of figure 6.3(d). This is done in figure 6.7 where the constituent functions u_n are shown together with the result from diagonalization. The agreement is excellent. The very small differences that remain are of course due to the fact that the delta function sum 6.55 is not the exact memory kernel.

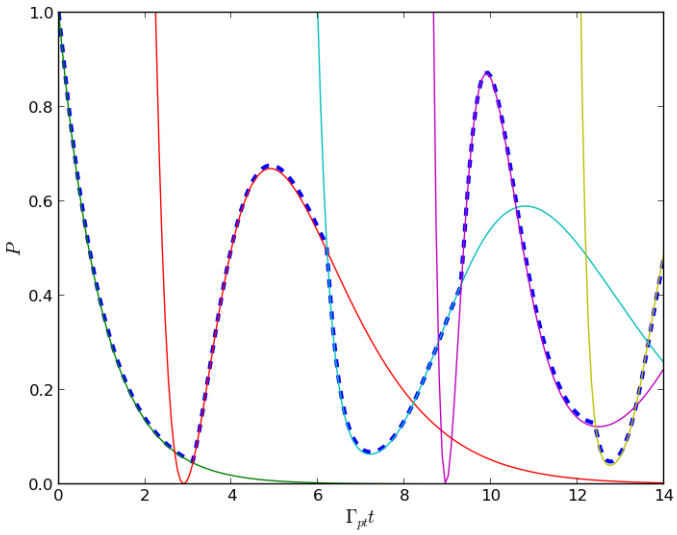


Figure 6.7: Development with an infinite sum of delta functions as approximation to the memory kernel is compared with exact numerical results. The constituent functions u_n of the approximate development are shown as the red, cyan, purple, yellow and black curve in increasing order of n. The exact result is the dashed blue curve. It is obtained with $\Delta\omega = N = 80$, and is identical to 6.3(d).

6.6.5 Numerical solution

We can also use the memory function approach to study the system when the timescale separation criterion is violated, and unlike the exact diagonalization approach this can be done without doing discrete approximations of the same dramatic nature. We do this by finding the exact memory kernel given some W, and then solving 6.36 exactly or numerically in some way. The way I have chosen to do this here is to make a Laplace transform: Letting $M(s)$ be the Laplace transform of the memory kernel and $a(s)$ that of $c(t)$, we take the Laplace transform of equation 6.36 to get

$$sa(s) - c(0) = M(s)a(s), \tag{6.62}$$

where we have used the rules for Laplace transforming derivatives and convolutions. Remembering that in our calculations $c(0) = 1$ we then get

$$a(s) = \frac{1}{s - M(s)}. \tag{6.63}$$

For a lot of different models this function is easy to calculate. However, in order to find $c(t)$ we must take the inverse Laplace transform of this. This can be done using the Mellin formula: $c(t) = \frac{1}{2\pi i}\int_l e^{st}a(s)ds$, with l a line in the imaginary direction laying to the right of all singularities of $a(s)$. Letting λ be the real coordinate of the line l (so that $s = \lambda + i\omega$ and $ds = id\omega$), the Mellin formula can be written out in terms of the inverse Fourier transform as $c(t) = e^{\lambda t}\mathcal{F}^{-1}(a(i\omega + \lambda))$. This is easy to implement numerically using an FFT algorithm. I have done this in Python, where this algorithm is available in a standard library. The values of λ are found using trial and error. That is to say: λ is simply increased until the solution stabilizes. As long as the memory function falls of sufficiently fast it can be set to zero.

The first we should do, given this new method of numerical analysis, is to verify that it agrees with the results of the diagonalization method. This is done in figure 6.8. In figure 6.8(a) and 6.8(b), the solution of 6.36 assuming a continuous flat W function with radius $\Delta\omega = 3\Gamma_{pt}$ is compared to 3 diagonalization results of the same model. These three calculations approximate the environment using 20, 40 and 80 oscillators.

In figure 6.8(a) the cyan curve is the memory equation result while the others are obtained by diagonalization. The results obtained using 20, 40 and 80 oscillators are shown as blue, red and green curves. In figure 6.8(a) the difference $P_D - P_M$ between the diagonalization and memory equation results is shown. The colors are the same. It is clear that the diagonalization result approaches the memory function result when the number of oscillators increases. This is what we would expect, since the continuous W function is better approximated with higher density of discrete oscillators.

To get a more direct comparison, we could solve 6.36 with the exact W function given the finite set of oscillators used for the diagonalization. This is what we see in figure 6.8(c) and 6.8(d). In 6.8(c) the two curves are compared directly, while in 6.8(d) the difference is again shown. The agreement between the curves is very good, but not perfect (The error is on the order of a few thousandths). This is because also the memory equation is solved numerically, so that in general the quality of the solution will depend on the resolution used in the FFT algorithm. In any case the figures seem to indicate that it is the memory equation approach that provides the most trustworthy results. This is also the one that can be applied over the longest time scales, as will be utilized in the next subsection.

6.6.6 Long time behavior

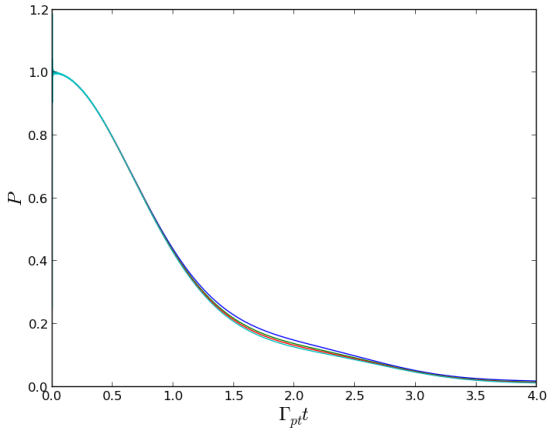
Finally, we will turn to the study of the systems behavior at long timescales. For this discussion we assume a continuous W function. This is something that is readily done by solving the memory equation 6.36, and also by diagonalization as long as a sufficiently high density of oscillators is used. A particularly interesting question is whether the evolution is asymptotically exponential. This is a question that applies both in the weakly and strongly interacting cases. In the weakly interacting cases we already know that the evolution is exponential over timescales comparable to the lifetime. But it is still a question whether it deviates from this at larger times. In the strongly interacting cases we see from for instance figure 6.4 that the evolution is not exponential in the time interval where most of the decay occurs, but it may still be so asymptotically.

One possible way of studying this question, is to look at the quantity $-\dot{P}/P$. If the evolution is asymptotically exponential, then this quantity should approach a constant value of Γ, the asymptotic decay rate. We do this analysis in figure 6.9 and 6.10, where the evolution given all four types of W functions discussed in section 6.6.3 is illustrated. In figure 6.9 the W function is assumed to be Gaussian or Lorenzian. As already discussed, in both these cases 6.40 has a solution. In figure 6.9 on the other hand, the W function is assumed to be flat or exponential ($\sim e^{-|\omega|/\Delta\omega}$), for which 6.40 does not have a solution.

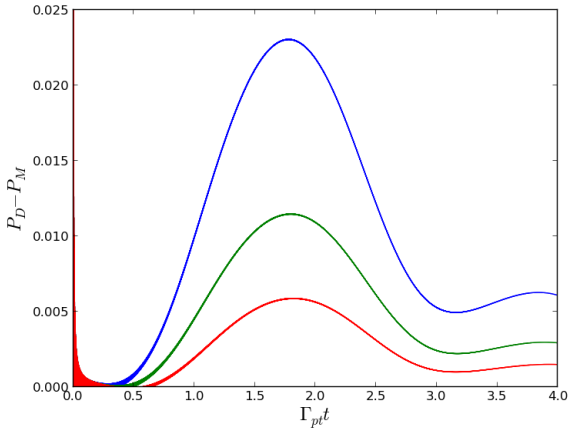
In both these figures I have shown the development according to both the diagonalization and memory equation methods, shown as blue and green curves respectively. In some of the plots the curves start to deviate from each other after some characteristic time. This is because it becomes to numerically demanding to include enough oscillators in the diagonalization to both include a sufficient width of the W function and also give correct behavior over long time scales. In these cases it is the longtime behavior of the memory equation result (green curve) that should be trusted.

The difference between the two figures is striking. In figure 6.9 all curves approach a constant value, strongly suggesting that we have an asymptotically exponential evolution. This happens both in the strongly interacting and weakly interacting cases. Indeed, the only differences seems to be that in the weak case the asymptotic decay rate is reached more or less immediately while in the strong case it takes some time, as well as the fact that the weak case value lies very close to 1 (in units of Γ_{pt}) while the strong case one lies somewhat higher.

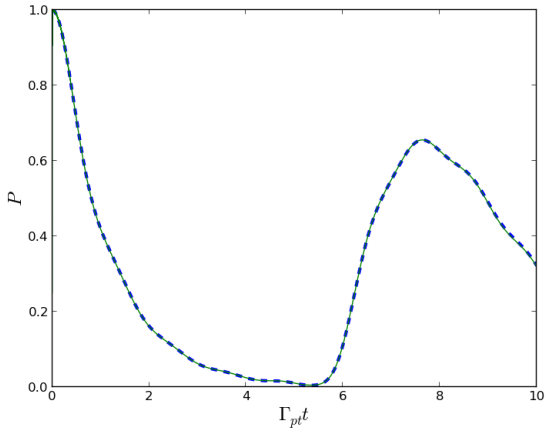
In figure 6.9 however, the situation is completely different. Here neither of the illustrated cases approach a constant value, indicating that we do not have asymptotically exponential behavior. With the flat W function the evolution of $-\dot{P}/P$ instead takes on a rapidly growing oscillatory behavior, while with the exponential one it simply keeps on growing. In the weakly interacting cases the rate stays around some intermediate approximately constant value for some amount of time, but then deviates from this later. In the strongly interacting cases the deviation happens more or less immediately.



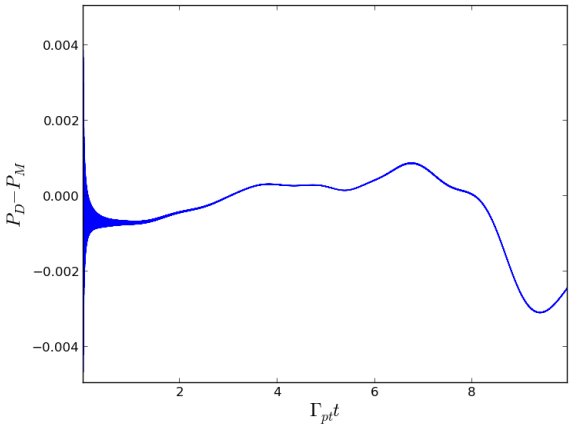
(a) Direct comparison. Continuous W function.



(b) Difference $P_D - P_M$. Continuous W function.

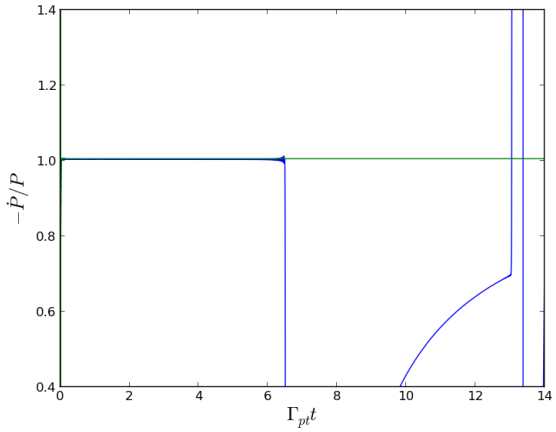


(c) Direct comparison. Discrete W function.

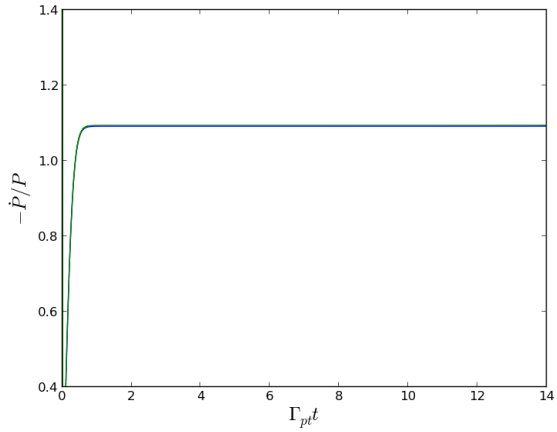


(d) Difference $P_D - P_M$. Discrete W function.

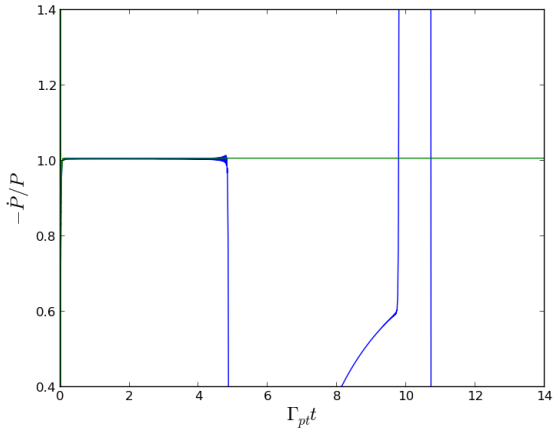
Figure 6.8: Comparison between numerical diagonalization result and solution to the memory equation 6.36. The memory equation is solved by taking the Laplace transform and its inverse numerically, as described in the text. In the upper figures the diagonalization result for 20, 40 and 80 oscillators is compared with the memory equation result with a flat continuous W function and $\Delta\omega = 3\Gamma_{pt}$. In the lower ones a diagonalization curve calculated with 10 oscillators is compared with the memory equation solution given the correct discrete W function resulting from that model. The figures to the left show direct comparisons of the obtained functions $P(t)$, while the ones to the right show the difference $P_D - P_M$ between the diagonalization and memory equation results. In 6.8(b) the memory equation result is the cyan curve, while in 6.8(d) it is the green, non-dashed one.



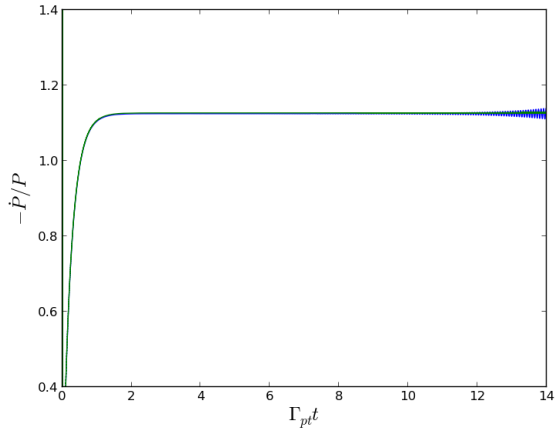
(a) Gaussian W function, $W = \hbar\Gamma_p t/80$.



(b) Gaussian W function, $W = \hbar\Gamma_p t/5$.

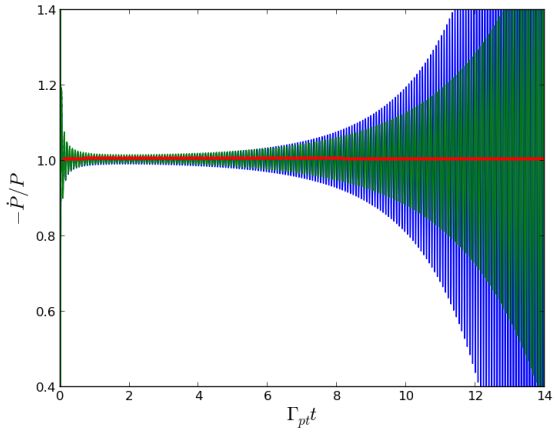


(c) Lorenzian W function, $W = \hbar\Gamma_p t/80$.

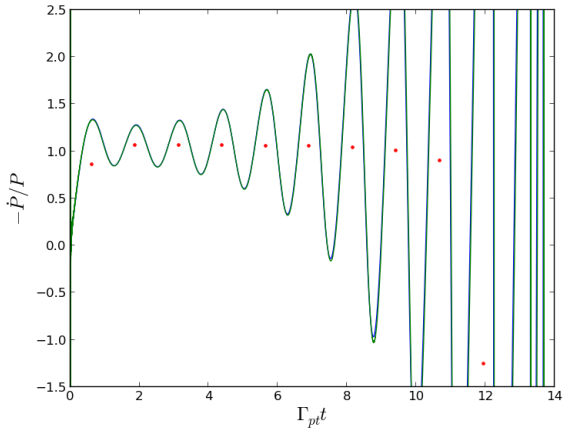


(d) Lorenzian W function, $W = \hbar\Gamma_p t/5$.

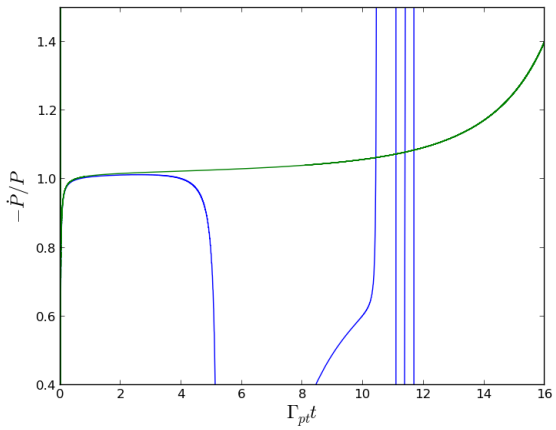
Figure 6.9: Longtime behavior of the quantity $-\dot{P}/P$ assuming a Gaussian or Lorenzian W function. The evolution is shown both in the weakly and strongly interacting cases, and is calculated using both the diagonalization (blue curve) and the memory equation method (green curve). As previously discussed, the diagonalization can not be trusted after some characteristic time $2\pi/\delta\omega$.



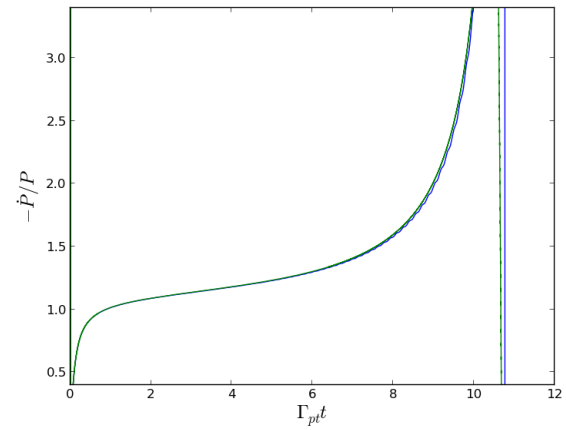
(a) Flat W function, $W = \hbar\Gamma_p t/80$.



(b) Flat W function, $W = \hbar\Gamma_p t/5$.



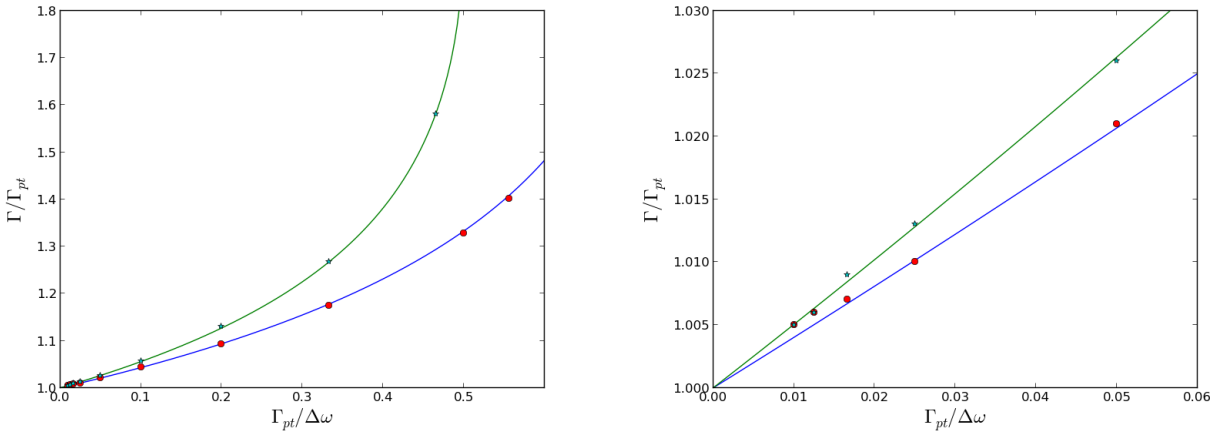
(c) Exponential W function, $W = \hbar\Gamma_p t/100$.



(d) Exponential W function, $W = \hbar\Gamma_p t/10$.

Figure 6.10: Longtime behavior of the quantity $-\dot{P}/P$ assuming a flat or exponential W function. The evolution is shown both in the weakly and strongly interacting cases, and is calculated using both the diagonalization (blue curve) and the memory equation method (green curve). In the flat model, strong oscillatory behavior is seen, so the average over periods of $2\pi/\Delta\omega$ are shown as red dots. As previously discussed, the diagonalization can not be trusted after some characteristic time $2\pi/\delta\omega$.

That only the models with Gaussian or Lorenzian W function converges to an asymptotic exponential decay is in well agreement with our previous discussion, which stated that the asymptotic evolution should be determined by equation 6.39. This equation does not have an exponential solution in the flat and exponential cases, whereas it does in the Gaussian and Lorenzian cases. The actual asymptotic rates in the numerical results can be found from simply reading of the value at which the plots stabilize. This should be compared with expressions found from solving 6.40, that is 6.48 in the Lorenzian case and the solution to 6.49 in the Gaussian case. This is done in figure 6.11, where again the agreement is excellent.



(a) All points

(b) Small values of $\Gamma_{pt}/\Delta\omega$

Figure 6.11: Comparison of asymptotic decay rates from simulations with expression found from solving 6.40. The green curve is this expression assuming a Lorenzian W function, while the blue assumes a Gaussian. The corresponding simulation results are shown as cyan and red marks respectively.

The results shown here strongly indicate that exponentially bounded memory kernels leads to exponential decay in the asymptotic limit. Also, it seems that we can expect deviations from exponential decay if the memory kernel is not exponentially bounded, just as was suggested by our earlier discussion. It has been shown[13][6] that if the range where the W function is nonzero has a lower bound (as will be the case in realistic physical systems since it is usually assumed that there are no negative energies), then the decay must proceed with a power law for sufficiently large times. It becomes an interesting question how this connects with our suspicion that the memory kernel must be exponentially bounded in order for the decay to be exponential.

Well, the memory kernel is related to the W-function by a Fourier transform. In fact, The claim of [13] is precisely that the Fourier transform of a function with limited support can not be asymptotically exponential. In this they refer to an original argument provided by [6]. This of course demonstrates that W functions of the mentioned type does not give rise to an exponential memory kernel. In [13] a very similar argument is used to argue directly that these W functions can not give rise to exponential decay: It is claimed that if the interactions does not have support over all frequencies, then neither can the Fourier transform of $c(t)$. Thus, $c(t)$ can not be asymptotically exponential.

6.7 Nakajima Zwanzieg Kernel

6.7.1 Calculation

As we see the exact memory equation for the probability amplitude $c(t)$ turns out to be very useful for the analysis of the two-level model. More complicated systems however can not be expected to be described by such a simple scalar equation with an exactly calculable Kernel. If we wish to analyze these with the memory kernel approach we must turn to the Nakajima Zwanzieg equation, and most likely to the perturbative expansion of its Kernel. Since this then is the method that best generalizes to other systems,

we should apply it also to the two-level model, since this would be the simplest possible application of that method.

Our first task is to calculate the first couple of orders in the memory kernel. In order to do this in an as simple way as possible, we first rewrite the interaction part of the Hamiltonian H_{SE} in the interaction picture as

$$H_{SE}(t) = \sum_i \left(w_i \sigma_+ \otimes a_i e^{-i(\omega_i - \omega)t} + w_i^\star \sigma_- \otimes a_i^\dagger e^{i(\omega_i - \omega)t} \right) = \sigma_+ \otimes B(t) + \sigma_- \otimes B(t)^\dagger, \text{ with} \tag{6.64}$$

$$B(t) = \sum_i w_i a_i e^{-i(\omega_i - \omega)t}, \tag{6.65}$$

with $\omega = E_0/\hbar$. We note that we have

$$B(t)\left|0\right\rangle = \sum_i w_i a_i(t)\left|0\right\rangle = 0, \text{ whereas} \tag{6.66}$$

$$B(t)B^\dagger(t')\left|0\right\rangle = \sum_{ij} w_i w_j^\star e^{-i(\omega_i-\omega)t + i(\omega_j-\omega)t'} a_i a_j^\dagger \left|0\right\rangle = \sum_i |w_i|^2 e^{-i(\omega_i-\omega)(t-t')}\left|0\right\rangle = -\hbar^2 K(t-t')\left|0\right\rangle, \tag{6.67}$$

where the last identity follows from noting that the function $\sum_i |w_i|^2 e^{-i(\omega_i-\omega)t}$ is the Fourier transform of the W function 6.7, and then simply applying 6.34.

For the two-level model, the super operator $\mathcal{L}(t)$ defined in the section on the Nakajima Zwanzieg formalism may now be expressed as

$$\mathcal{L}(t)\rho = -\frac{i}{\hbar}[H_{SE}, \rho] = -\frac{i}{\hbar}((\sigma_+ \otimes B(t))\rho + (\sigma_- \otimes B(t)^\dagger)\rho - \rho(\sigma_+ \otimes B(t)) - \rho(\sigma_- \otimes B^\dagger(t))), \tag{6.68}$$

and with this we are ready to calculate the different orders of the memory kernel.

We begin by noting that 6.66 implies that the condition $\mathrm{Tr}_E \mathcal{L}(t)\rho_S \otimes \left|0\right\rangle\left\langle 0\right| = 0$ is satisfied. This was a requirement for the version of the Nakajima Zwanzieg equation derived in section 5 to be valid (see eq. 5.2). In fact it is easily seen that this result also generalizes to similar expressions involving any odd power of the Liouville operators. This can be written as $\mathcal{P}\mathcal{L}(t_1)\cdots\mathcal{L}(t_{2n+1})\mathcal{P} = 0$, which further implies that $\mathcal{Q}\mathcal{L}(t_1)\cdots\mathcal{L}(t_{2n+1})\mathcal{P} = \mathcal{L}(t_1)\cdots\mathcal{L}(t_{2n+1})\mathcal{P}$. This means all odd orders of 5.14 are 0. Also, any $\mathcal{Q}$ operator in the expression that has an odd number of $\mathcal{L}$ operators between it self and the $\mathcal{P}$ operators will disappear. This fact will be used in the following calculations. Even so, these calculations will be quite involved. The reader is duly warned.

Using 6.68 and 6.66 as well as the fact that $\sigma_-^2 = \sigma_+^2 = 0$ and $\sigma_+\sigma_- = P_e$ we get

$$\begin{aligned}
\mathcal{L}(t)\mathcal{L}(t')\rho_S \otimes \left|0\right\rangle\left\langle 0\right| =& \mathcal{L}(t)(\sigma_-\rho_S \otimes B^\dagger(t')\left|0\right\rangle\left\langle 0\right| - \rho_S\sigma_+ \otimes \left|0\right\rangle\left\langle 0\right| B(t')) \\
=& P_e\rho_S \otimes B(t)B^\dagger(t')\left|0\right\rangle\left\langle 0\right| - \sigma_-\rho_S\sigma_+ \otimes B^\dagger(t')\left|0\right\rangle\left\langle 0\right| B(t) \\
& - \sigma_-\rho_S\sigma_+ \otimes B^\dagger(t)\left|0\right\rangle\left\langle 0\right| B(t') + \rho_S P_e \otimes \left|0\right\rangle\left\langle 0\right| B(t')B^\dagger(t) \\
=& P_e\rho_S \otimes K(t-t')\left|0\right\rangle\left\langle 0\right| - \sigma_-\rho_S\sigma_+ \otimes B^\dagger(t')\left|0\right\rangle\left\langle 0\right| B(t) \\
& - \sigma_-\rho_S\sigma_+ \otimes B^\dagger(t)\left|0\right\rangle\left\langle 0\right| B(t') + \rho_S P_e \otimes \left|0\right\rangle\left\langle 0\right| K(t'-t).
\end{aligned} \tag{6.69}$$

And applying the super operator $\mathcal{P}$ to this, we get the lowest order term in the memory kernel:

$$\begin{aligned}\mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\rho_S\otimes|0\rangle\langle 0| =&(P_e\rho_S K(t-t') - \sigma_-\rho_S\sigma_+ \mathrm{Tr}B^\dagger(t')|0\rangle\langle 0|B(t)\\ &-\sigma_-\rho_S\sigma_+\mathrm{Tr}B^\dagger(t)|0\rangle\langle 0|B(t') + \rho_S P_e K(t'-t))\otimes|0\rangle\langle 0|\\ =&(P_e\rho_S K(t-t') - \sigma_-\rho_S\sigma_+\langle 0|B(t)B^\dagger(t')|0\rangle\\ &-\sigma_-\rho_S\sigma_+\langle 0|B(t')B^\dagger(t)|0\rangle + \rho_S P_e K(t'-t))\otimes|0\rangle\langle 0|\\ =&(P_e\rho_S K(t-t') + \rho_S P_e K(t'-t) - \sigma_-\rho_S\sigma_+(K(t-t')+K(t'-t)))\otimes|0\rangle\langle 0|\end{aligned} \tag{6.70}$$

Using this as well as the above mentioned expressions, it is also easy to calculate

$$\begin{aligned}\mathcal{Q}\mathcal{L}(t)\mathcal{L}(t')\rho_S\otimes|0\rangle\langle 0| &= \mathcal{L}(t)\mathcal{L}(t')\rho_S\otimes|0\rangle\langle 0| - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\rho_S\otimes|0\rangle\langle 0|\\ &= \sigma_-\rho_S\sigma_+\otimes((K(t-t')+K(t'-t))|0\rangle\langle 0| - B^\dagger(t')|0\rangle\langle 0|B(t) - B^\dagger(t)|0\rangle\langle 0|B(t'))\end{aligned} \tag{6.71}$$

and further

$$\begin{aligned}&\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{Q}\mathcal{L}(t_2)\mathcal{L}(t')\rho_S\otimes|0\rangle\langle 0| =\\ &\mathcal{L}(t)\mathcal{L}(t_1)(\sigma_-\rho_S\sigma_+\otimes((K(t_2-t')+K(t'-t_2))|0\rangle\langle 0| - B^\dagger(t')|0\rangle\langle 0|B(t_2) - B^\dagger(t_2)|0\rangle\langle 0|B(t'))) =\\ &\mathcal{L}(t)(-P_e\rho_S\sigma_+K(t_1-t')\otimes|0\rangle\langle 0|B(t_2) + \sigma_-\rho_S P_e\otimes B^\dagger(t')|0\rangle\langle 0|K(t_2-t_1)\\ &-P_e\rho_S\sigma_+K(t_1-t_2)\otimes|0\rangle\langle 0|B(t') + \sigma_-\rho_S P_e\otimes B^\dagger(t_2)|0\rangle\langle 0|K(t'-t_1)) =\\ &-\sigma_-\rho_S\sigma_+K(t_1-t')\otimes B^\dagger(t')|0\rangle\langle 0|B(t_2) + P_e\rho_S P_e K(t_1-t')K(t_2-t)\otimes|0\rangle\langle 0|\\ &+P_e\rho_S P_e K(t-t')K(t_2-t_1)\otimes|0\rangle\langle 0| - \sigma_-\rho_S\sigma_+K(t_2-t_1)\otimes B^\dagger(t')|0\rangle\langle 0|B(t) + \text{h.c.},\end{aligned} \tag{6.72}$$

where h.c. signifies the Hermitian conjugate, or adjoint operator of the entire preceding expression. For the last step it is necessary to apply the fact that $K(t) = K(-t)^\star$, which follows from 6.34 together with the reality of W.

The next, fourth order term in the memory kernel can be found from this by once again applying the super operator $\mathcal{P}$ and then performing the appropriate integrals, as seen in 5.14. However, since we are interested in a memory equation for ρ_S not $\rho_S\otimes|0\rangle\langle 0|$ it is enough to apply Tr_E rather than $\mathcal{P}$:

$$\begin{aligned}&\mathrm{Tr}_E\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{Q}\mathcal{L}(t_2)\mathcal{L}(t')\rho_S\otimes|0\rangle\langle 0| =\\ &-\sigma_-\rho_S\sigma_+K(t_1-t')\langle 0|B(t_2)B^\dagger(t')|0\rangle + P_e\rho_S P_e K(t_1-t')K(t_2-t)\otimes|0\rangle\langle 0|\\ &+P_e\rho_S P_e K(t-t')K(t_2-t_1) - \sigma_-\rho_S\sigma_+K(t_2-t_1)\langle 0|B(t)B^\dagger(t')|0\rangle + \text{h.c.}, =\\ &-\sigma_-\rho_S\sigma_+K(t_1-t')K(t_2-t') + P_e\rho_S P_e K(t_1-t')K(t_2-t)\\ &+P_e\rho_S P_e K(t-t')K(t_2-t_1) - \sigma_-\rho_S\sigma_+K(t_2-t_1)K(t-t') + \text{h.c.}\end{aligned} \tag{6.73}$$

Utilizing this and 6.70 we see that the Nakajima Zwanzieg memory kernel of the two-level model is given by

$$\begin{aligned}\mathcal{K}(t,t')\rho_S =&P_e\rho_S K(t-t') - \sigma_-\rho_S\sigma_+K(t-t')+\\ &(P_e\rho_S P_e - \sigma_-\rho_S\sigma_+)\int_{t'}^{t}\int_{t'}^{t_1}(K(t-t')K(t_2-t_1)+K(t_1-t')K(t_2-t))dt_2dt_1\\ &+\text{h.c.} + 6.\text{ and higher order terms.}\end{aligned} \tag{6.74}$$

The 5. order terms are zero like all other odd terms. We could easily have continued in the manner above to find for instance the sixth and eight order contributions. However, due to issues of time and space this will not be done. Instead we note a general trend, namely that all higher order contributions will consist of terms proportional to the operators $P_e\rho_S P_e$ or $\sigma_-\rho_S\sigma_+$. This can bee seen by noting that the fourth order terms in 6.72 are of this form, and that all higher order terms results from applying σ_- or σ_+ twice to the right or left of a term of order two less. The only non zero operators that can result from doing this to $P_e\rho_S P_e$ or $\sigma_-\rho_S\sigma_+$ are themselves proportional to these operators. It then follows through induction that all higher order terms must have this form.

6.7.2 Discussion

We may use 6.74 to find equations for the individual components of ρ_S. We see however from 6.25 that ρ_S actually only has two independent parameters, which could for instance be taken to be ρ_{12} and $P = \rho_{11}$. Note that this generalizes to any two state system. The equations for these two quantities are obviously given by

$$\dot{\rho}_{12} = \langle e|\, \dot{\rho}_S\, |g\rangle = \int_0^t \langle e|\, \mathcal{K}(t,t')\rho_S\, |g\rangle\, dt', \tag{6.75}$$

$$\dot{P} = \langle e|\, \dot{\rho}_S\, |e\rangle = \int_0^t \langle e|\, \mathcal{K}(t,t')\rho_S\, |e\rangle\, dt'. \tag{6.76}$$

That is, they satisfy two memory equations themselves. In general these equations may obviously be coupled, but in this model we will see that they are not. In fact, from the expression for ρ_{12} in 6.25 we see that this quantity will satisfy precisely the same memory equation as $c(t)$, and so we would expect the memory kernel of 6.75 to simply be $K(t-t')$. Let us check if this is the case by evaluating the matrix element $\langle e|\, \mathcal{K}(t,t')\rho_S\, |g\rangle$.

We begin by noting that all terms in $\mathcal{K}(t,t')\rho_S$ are proportional to either $P_e\rho_S$, $\rho_S P_e$, $P_e\rho_S P_e$ or $\sigma_-\rho_S\sigma_+$. By the argument above this also applies to terms of higher order than 4. It is easily seen that $\langle e|\, P_e\rho_S P_e\, |g\rangle = \langle e|e\rangle\, \langle e|\, \rho_S\, |e\rangle\, \langle e|g\rangle = 0$ and $\langle e|\, \sigma_-\rho_S\sigma_+\, |g\rangle = \langle e|g\rangle\, \langle e|\, \rho_S\, |e\rangle\, \langle g|g\rangle = 0$. Since these are the only terms contained in the higher order contributions, the entire contribution to $\langle e|\, \mathcal{K}(t,t')\rho_S\, |g\rangle$ must come from the second order terms proportional to $P_e\rho_S$ and $\rho_S P_e$. Now $\langle e|\, \rho_S P_e\, |g\rangle = \langle e|\, \rho_S\, |e\rangle\, \langle e|g\rangle = 0$, so this does not contribute either. The contribution from $\rho_S P_e$ on the other hand is $\langle e|\, P_e\rho_S\, |g\rangle = \langle e|e\rangle\, \langle e|\, \rho_S\, |g\rangle = \rho_{12}$, the only non zero contribution. Thus we see that in fact $\langle e|\, \mathcal{K}(t,t')\rho_S\, |g\rangle = K(t-t')\rho_{12}$, and 6.75 becomes a memory equation in ρ_{12} alone, with $K(t-t')$ as its memory kernel precisely as we expected.

Let us now turn to the equation for P, and calculate the expression $\langle e|\, \mathcal{K}(t,t')\rho_S\, |e\rangle$. We first note that $\langle e|\, \sigma_-\rho_S\sigma_+\, |e\rangle = \langle e|g\rangle\, \langle e|\, \rho_S\, |e\rangle\, \langle g|e\rangle = 0$, so that these terms again does not contribute. In much the same way we calculate $\langle e|\, P_e\rho_S\, |e\rangle = \langle e|\, \rho_S P_e\, |e\rangle = \langle e|\, P_e\rho_S P_e\, |e\rangle = P$, which means that

$$\begin{aligned}\langle e|\, \mathcal{K}(t,t')\rho_S\, |e\rangle =& K(t-t')P + P\int_{t'}^t\int_{t'}^{t_1} (K(t-t')K(t_2-t_1) + K(t_1-t')K(t_2-t))dt_2dt_1 \\ &+ \text{c.c.} + 6.\text{ and higher order terms,}\end{aligned} \tag{6.77}$$

where c.c. signifies the complex conjugate of the entire preceding expression. Thus to the fourth order we see from 6.75 that $P(t)$ satisfies the uncoupled memory equation

$$\dot{P}(t) = \int_0^t K_P(t,t')P(t')dt', \text{ with} \tag{6.78}$$

$$K_P(t,t') = K(t-t') + \int_{t'}^t\int_{t'}^{t_1} (K(t-t')K(t_2-t_1) + K(t_1-t')K(t_2-t))dt_2dt_1 + \text{c.c.} \tag{6.79}$$

We note that if we go only to the second order, the memory kernel $K_P(t,t')$ for $P(t) = |c(t)|^2$ is just twice the real part of $K(t-t')$, which is the memory kernel for $c(t)$.

Just to verify that the Nakajima Zwanzieg equation makes sense, we may also calculate the expression for $\dot{\rho}_{22}$. This will be an expression of precisely the same form as 6.75, except involving the quantity $\langle g| \mathcal{K}(t,t')\rho_S |g\rangle$. In the same manner as above it is easily seen that operators of type $P_e\rho_S$, $\rho_S P_e$ and $P_e\rho_S P_e$ all give contribution zero to this expression, whereas $\langle g| \sigma_-\rho_S\sigma_+ |g\rangle = \langle g|g\rangle \langle e| \rho_S |e\rangle \langle g|g\rangle = P$. Thus, from 6.74 we see that $\langle g| \mathcal{K}(t,t')\rho_S |g\rangle = -\langle e| \mathcal{K}(t,t')\rho_S |e\rangle$ given by 6.77. Clearly then $\dot{\rho}_{22} = -\dot{\rho}_{11}$, which is in complete agreement with 6.25 and common sense in general.

We would now like to know whether 6.78 is in agreement with the memory equation for $c(t)$. There is one obvious way of doing this: We numerically solve the memory equation for $c(t)$ just like in the previous section, calculate $P(t) = |c(t)|^2$, and compare this with the numerical solution of 6.78. In order to do this however we must find a way to efficiently calculate the memory kernel $K_P(t,t')$, which involves a double integral.

We do this by first re-expressing the integrals using the following definitions: given functions $f(t)$ and $g(t)$ we define new functions f_1, f_2 and $f \star g$ as

$$f_1(t) = \int_0^t f(t')dt', \tag{6.80}$$

$$f_2(t) = \int_0^t f_1(t')dt', \tag{6.81}$$

$$(f \star g)(t) = \int_0^t f(t')g(t-t')dt' = \int_0^t f(t-t')g(t')dt', \tag{6.82}$$

which have the advantage of being defined through operations that can be efficiently implemented in Python. Given these definitions, we may re-express the double integral in 6.77 as

$$\int_{t'}^t \int_{t'}^{t_1} (K(t-t')K(t_2-t_1) + K(t_1-t')K(t_2-t))dt_2dt_1 =$$

$$\int_{t'}^t \int_{t'}^{t_1} (K(t-t')K^\star(t_1-t_2) + K(t_1-t')K^\star(t-t_2))dt_2dt_1 =$$

$$\int_{t'}^t (K(t-t')(K_1^\star(t_1-t_1) - K_1^\star(t_1-t')) + K(t_1-t')(K_1^\star(t-t_1) - K_1^\star(t-t')))dt_1 =$$

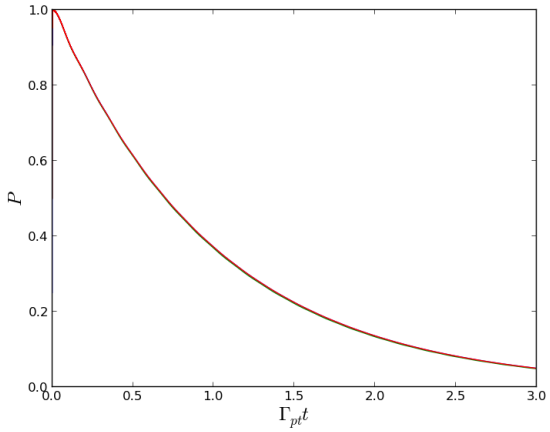
$$-K(t-t')\int_{t'}^t K_1^\star(t_1-t')dt_1 + \int_{t'}^t K(t_1-t')K_1^\star(t-t_1)dt_1 - K_1^\star(t-t')\int_t^{t'} K(t_1-t')dt_1 =$$

$$-K(t-t')K_2^\star(t-t') + \int_0^{t-t'} K(u)K_1^\star(t-t'-u)du - K_1^\star(t-t')K_1(t-t') =$$

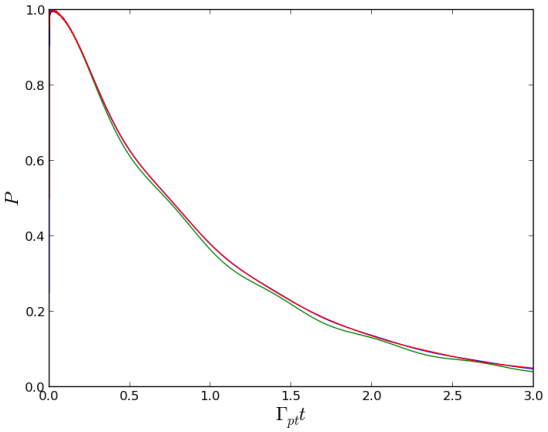
$$-K(t-t')K_2^\star(t-t') + (K \star K_1^\star)(t-t') - |K_1(t-t')|^2 =$$

$$(K \star K_1^\star - K \cdot K_2^\star - |K_1|^2)(t-t'). \tag{6.83}$$

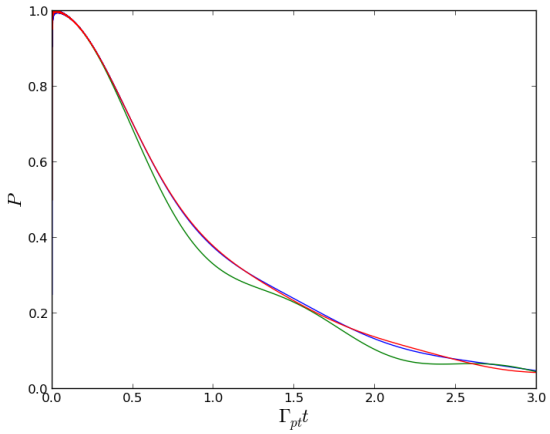
In addition to being efficiently implementable, this expression also demonstrates that to the fourth order $K_P(t,t')$ is just like K a function only of the distance $t-t'$. This means that we can solve the memory equation for P in precisely the same manor as we did the one for c, namely through a Laplace transform. See the previous section for more details. In figure 6.12 we see the function $P(t)$ as calculated from the exact formula $P = |c|^2$ compared with the results of solving 6.78. Both the second and fourth order approximation of K_P is used.



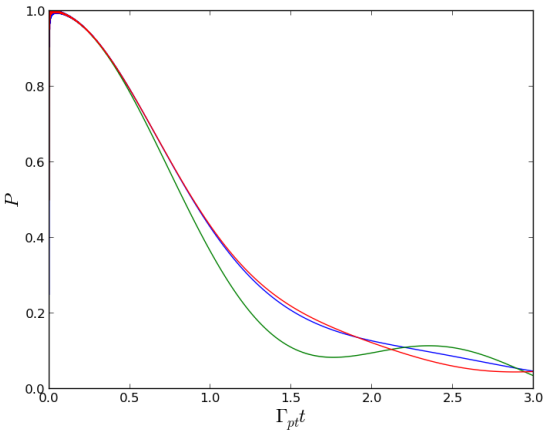
(a) $\Delta E = 40\hbar\Gamma$.



(b) $\Delta E = 10\hbar\Gamma$.



(c) $\Delta E = 5\hbar\Gamma$.



(d) $\Delta E = 3\hbar\Gamma$.

Figure 6.12: Comparison of $P(t)$ as calculated by solving the exact memory equation for $c(t)$ (blue curve) with the same quantity calculated by solving the second (green curve) and fourth order (red curve) approximations to the Nakajima Zwanzieg equation. Note how for decreasing value of $\Delta E/\hbar\Gamma$ we first get a notable deviation between the exact result and the second order approximation, while the fourth order approximation only deviates notably at even smaller values of this parameter.

6.8 Expansion of the Markovian generator

6.8.1 Calculation

In the section on general non-Markovian descriptions I mentioned that given some memory equation, then provided the development is invertible one can find an exact Markovian generator that can be expanded as 5.24. In that chapter we applied this to the general Nakajima Zwanzieg equation in order to find the general expansion 5.25 of the Markovian generator of the state operator of open systems. This expansion could have been applied to the two-level model if we wished an approximation to this generator that is more accurate than the Lindblad/Redfield approximation used earlier in the chapter. However, with this particular model we can take a different approach. Since the system is in this case completely described by the simple scalar memory equation 6.36, and this equation even has an exactly calculable kernel, it is much simpler to just apply 5.24 to this instead. To see 5.25 applied to this model, see [2].

With the specific scalar memory kernel $K(t-t')$, 5.24 becomes

$$m(t) = \sum_{n=0}^{\infty} \int_0^t \int_t^{t'} \int_0^{t_1} \int_t^{t'_1} \cdots \int_t^{t'_{n-1}} \int_0^{t_n} K(t-t')K(t_1-t'_1)\cdots K(t_n-t'_n)dt'_n dt_n \cdots dt'_1 dt_1 dt', \quad (6.84)$$

where $m(t)$ is the Markovian generator of $c(t)$. We can write this more systematically by first defining the quantities $m_n(t,t')$ recursively as

$$m_1(t,t') = \int_0^t K(s)ds, \text{ and} \quad (6.85)$$

$$\begin{aligned} m_n(t,t') &= \int_0^t \int_{t'}^{s} K(t-s)m_{n-1}(s',t')ds'ds \\ &= \int_0^t K(s) \int_{t'}^{t-s} m_{n-1}(s',t')ds'ds, \text{ for } n>1. \end{aligned} \quad (6.86)$$

I is not hard to convince one self that 6.84 can then be written simply as

$$m(t) = \sum_{n=1}^{\infty} m_n(t,t). \quad (6.87)$$

This systematic rewriting of the expansion in principle enables us to recursively calculate the terms of $m(t)$. However, due to the two dimensional nature of the functions $m_n(t,t')$ this is not numerically very efficient: We would be required to store a 2 dimensional array of function values, which would have a great impact on the memory requirements and calculation time. This would probably have meant that accuracy would have to sacrificed in order to decrease these requirements. Thus, in order to end up with the numerically most efficient calculation, we continue our rewriting: First, we define the quantities $l_n(t)$ through formulas very similar to 6.85 and 6.86:

$$l_1(t) = m_1(t,t') = \int_0^t K(s)ds, \text{ and} \quad (6.88)$$

$$l_n(t) = \int_0^t K(s) \int_0^{t-s} l_{n-1}(s')ds'ds, \text{ for } n>1. \quad (6.89)$$

It turns out that the fucnctions $m_n(t,t')$ can be be defined through the functions $l_n(t)$ as

$$m_n(t,t') = l_n(t) - \sum_{j=1}^{n-1} l_j(t) \int_0^{t'} m_{n-j}(s,t')ds. \quad (6.90)$$

To prove this we first note that this is obviously true in the $n = 1$ case, and then we prove that it is true in any case n if it is true for $n - 1$. This can be done by the following calculation:

$$\begin{aligned}
m_n(t,t') &= \int_0^t K(s) \int_{t'}^{t-s} m_{n-1}(s',t')ds'ds \\
&= \int_0^t K(s) \int_0^{t-s} m_{n-1}(s',t')ds'ds - \int_0^t K(s) \int_0^{t'} m_{n-1}(s',t')ds'ds \\
&= \int_0^t K(s) \int_0^{t-s} \left(l_{n-1}(s') - \sum_{j=1}^{n-2} l_j(s') \int_0^{t'} m_{n-1-j}(u,t')du \right) ds'ds - l_1(t) \int_0^{t'} m_{n-1}(s',t')ds' \\
&= l_n(t) - \sum_{j=1}^{n-2} \int_0^t K(s) \int_0^{t-s} l_j(s')ds'ds \int_0^{t'} m_{n-1-j}(u,t')du - l_1(t) \int_0^{t'} m_{n-1}(s',t')ds' \\
&= l_n(t) - \sum_{j=1}^{n-2} l_{j+1}(t) \int_0^{t'} m_{n-1-j}(u,t')du - l_1(t) \int_0^{t'} m_{n-1}(s',t')ds' \\
&= l_n(t) - \sum_{j=1}^{n-1} l_j(t) \int_0^{t'} m_{n-j}(u,t')du. \qquad (6.91)
\end{aligned}$$

Having now proven 6.90, we now make the definitions

$$m_n(t) = m_n(t,t), \qquad (6.92)$$

$$\bar{m}_n(t) = \int_0^t m_n(s,t)ds \text{ and} \qquad (6.93)$$

$$\bar{l}_n(t) = \int_0^t l_n(s)ds. \qquad (6.94)$$

This makes us able to sum up our results as

$$m(t) = \sum_{n=1}^{\infty} m_n(t), \text{ with} \qquad (6.95)$$

$$m_n(t) = l_n(t) - \sum_{j=1}^{n-1} l_j(t)\bar{m}_{n-j}(t), \qquad (6.96)$$

$$\bar{m}_n(t) = \bar{l}_n(t) - \sum_{j=1}^{n-1} \bar{l}_j(t)\bar{m}_{n-j}(t), \qquad (6.97)$$

$$l_n(t) = \int_0^t K(s) \int_0^{t-s} l_{n-1}(s')ds'ds \text{ for } n > 1, \qquad (6.98)$$

$$\bar{l}_n(t) = \int_0^t l_n(s)ds \text{ and} \qquad (6.99)$$

$$l_1(t) = \int_0^t K(s)ds. \qquad (6.100)$$

Clearly this representation looks much more complicated and cumbersome than 6.85 to 6.87. The equations 6.95 to 6.100 however have the advantage of only involving one dimensional functions, which

dramatically reduces the memory requirements. Also, the only operation that scales more than linearly is 6.98, which can actually be written as $l_n = K \star (l_{n-1})_1$ using the notation that was defined in the previous section. As already mentioned these operations are efficiently implemented in Python, and thus the entire calculation can be done very fast and efficiently.

6.8.2 Discussion

Since $m(t)$ is its Markovian generator, $c(t)$ obeys the equation $\dot{c}(t) = m(t)c(t)$. This equation has a very simple solution, namely $c(t) = c(0)e^{\int_0^t m(s)ds}$. Also, $P(t) = |c(t)|^2$ obeys the equation $\dot{P}(t) = 2\mathcal{R}e\, m(t)c(t)$, with the equally simple solution $P(t) = P(0)e^{2\mathcal{R}e\int_0^t m(s)ds}$. This is actually an equation we have seen before, in the chapter on Redfield formalism. There however, $m(t)$ was the Redfield approximation, and given by $-\Gamma(t)$ from 6.20. If we take into account 6.34 we should recognize this expression as being the first order term $m_1(t)$ of the expansion 6.95. We noted earlier that 6.22 is not an exact solution, and we understand now that this is because it only includes the first order term in this expansion. By including more terms we should be able to improve upon the results. This is examined in figure 6.13.

We see that when $\Delta E = 3\hbar\Gamma$ the second order curve is definitely a better approximation to the exact result than the 1. order curve, which is the Redfield solution. In fact, if we go to the 3. order, the curve is nearly indistinguishable from the exact result. In the $\Delta E = 2\hbar\Gamma$ and $\Delta E = \hbar\Gamma$ cases we must go to even higher orders to get near perfect correspondence with the exact result. The results are only included up to the 5. order due to numerical instabilities in the higher orders.

In any case the figures seem to indicate that for the three first values of $\Delta E/\hbar\Gamma$ we have convergence towards the exact curve as $n \to \infty$. For the last value however, that is $\Delta E = \frac{1}{2}\hbar\Gamma$, this is clearly not the case. In this figure the exact result reaches 0 at $\Gamma t \approx 4.1$, and then rises again to make a small bulk. None of the Markovian curves show this behavior, and it seems the Markovian expansion does not at all converge to the correct value after this point.

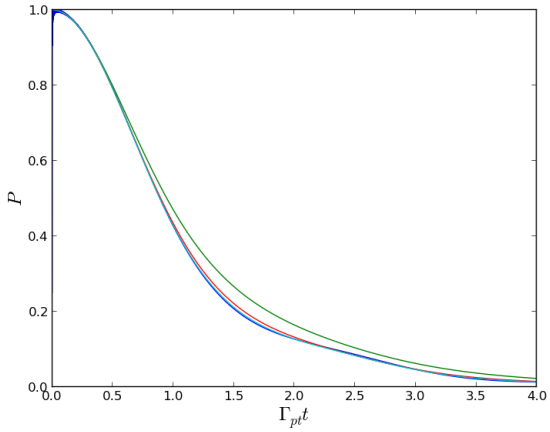
This is not a mystery, but in fact has a very natural explanation and makes a good illustration of a very important point: It was stated in chapter 5 that it is a prerequisite for the existence of an exact Markovian generator that the time development of the system is invertible in the entire interval where it is calculated. In this case the time development is represented by the simple scalar function $c(t)$, which is *zero* at $t \approx 4.1$ and thus not invertible. The exact Markovian generator thus only exists in the interval $[0, 4.1]$, where indeed the expansion results still seem to converge nicely.

After $t \approx 4.1$ there is not really any Markovian generator to expand, and thus we should not be surprised when such an expansion does in fact not work! For times larger than 4.1 this is clearly an example of a system that is truly non-Markovian, in that there exists no Markovian generator that is capable of describing it. Such a system can only be described using a memory equation or some other explicitly non-Markovian technique.

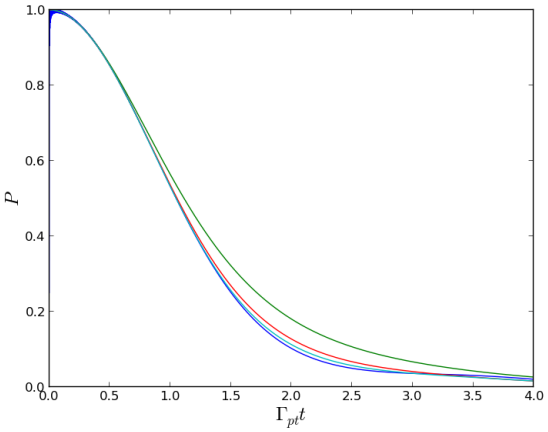
To examine the convergence of the Markovian generator in the clearest possible way, it is better to compare $2\mathcal{R}e\, m(t)$ directly with $\dot{P}/P$. This allows us to see all the details in $m(t)$ without the exponential damping, and thus allows us to study for instance the asymptotic behavior. It also makes us able to distinguish the characteristics of different types of W functions. This is illustrated in figure 6.14 and 6.15, using W functions similar to those of figure 6.9 and 6.10.

These figures should demonstrate even clearer than figure 6.13 how well the Markovian expansion actually works. Let us first discuss figure 6.14, where the exact result seems to approach an asymptotic decay rate. First of all, all the expansion curves are in agreement with this, as they also approach some asymptotic value. For modestly weak interactions ($\Delta E = 10\hbar\Gamma$), the expansion result is nearly inseparable from the exact result already at the second order. In the case of quite strong interactions ($\Delta E = 2\hbar\Gamma$) and a Gaussian W function one must go to the fifth order before this becomes true. However, in the same strong interaction case but with a Lorenzian W function, the expansion curves have not converged to the exact result even after 6 orders.

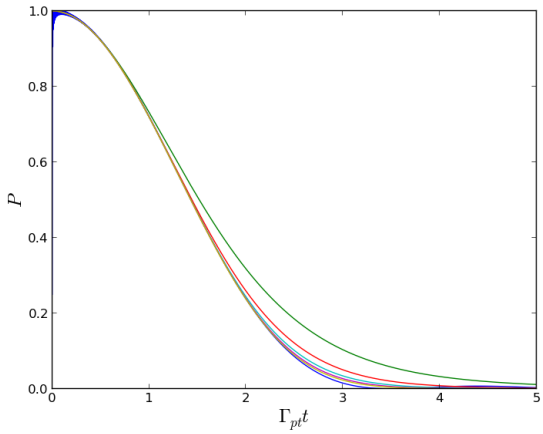
I have not included any more than 6 orders in that figure, since from the 7.order and onwards they showed signs of great numerical instability. The curves do however seem to be on their way to converging,



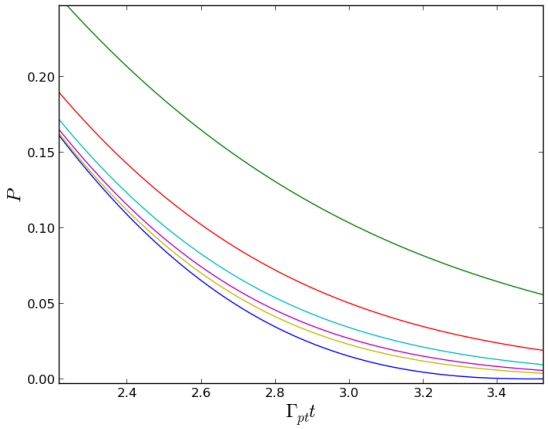
(a) $\Delta E = 3\hbar\Gamma$.



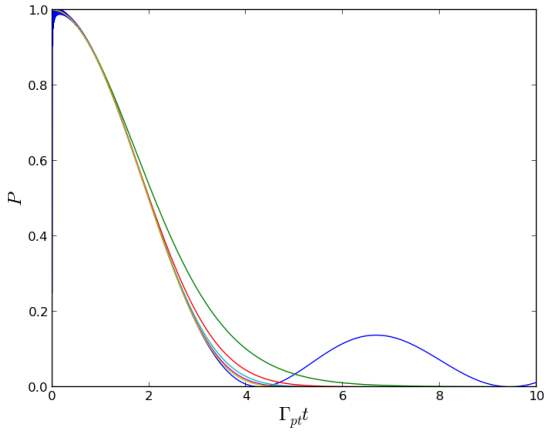
(b) $\Delta E = 2\hbar\Gamma$.



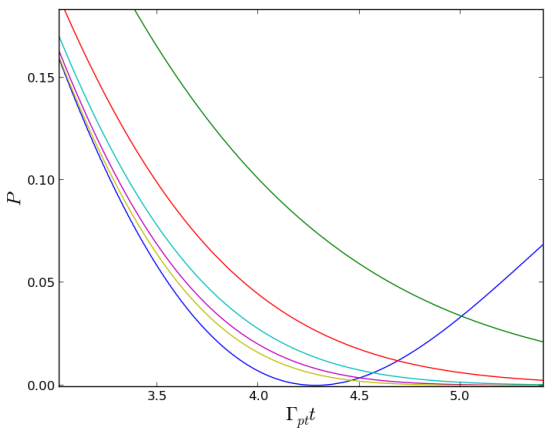
(c) $\Delta E = \hbar\Gamma$.



(d) $\Delta E = \hbar\Gamma$, details.

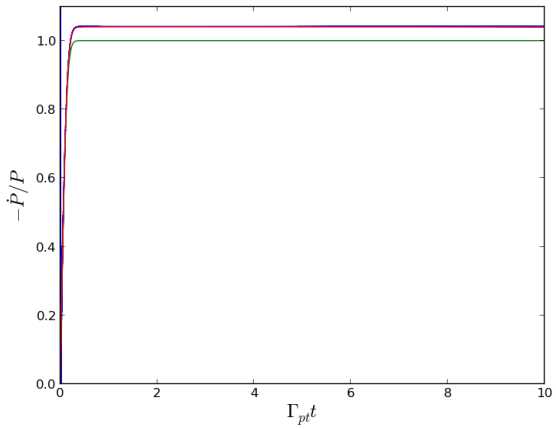


(e) $\Delta E = \frac{1}{2}\hbar\Gamma$.

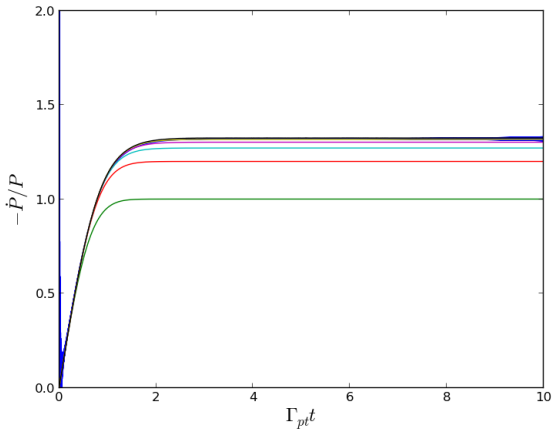


(f) $\Delta E = \frac{1}{2}\hbar\Gamma$, details.

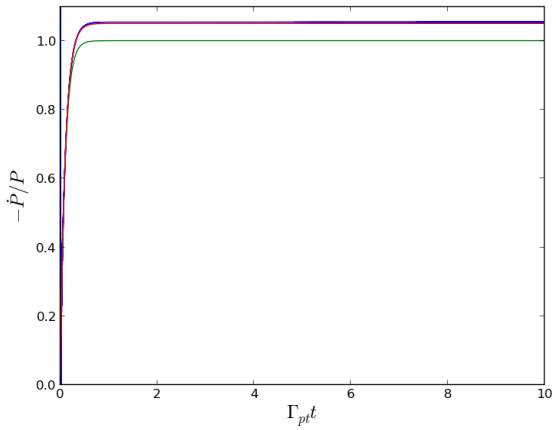
Figure 6.13: $P(t)$ as calculated through the solution of the exact equation 6.36, compared with results obtained using a Markovian generator calculated to various orders (using 6.95). The exact result is the blue curve, while the 1., 2., 3., 4., and 5. order results are shown as green, red, cyan, purple and yellow curves respectively.



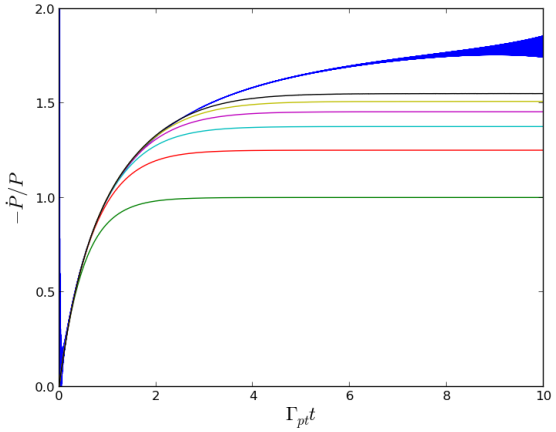
(a) Gaussian W, $\Delta E = 10\hbar\Gamma$.



(b) Gaussian W, $\Delta E = 2\hbar\Gamma$.

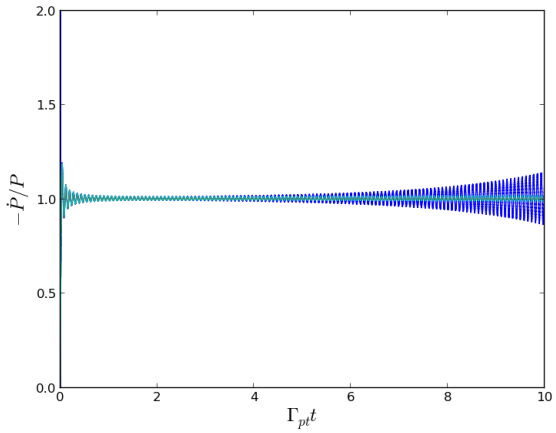


(c) Lorenzian W, $\Delta E = 10\hbar\Gamma$.

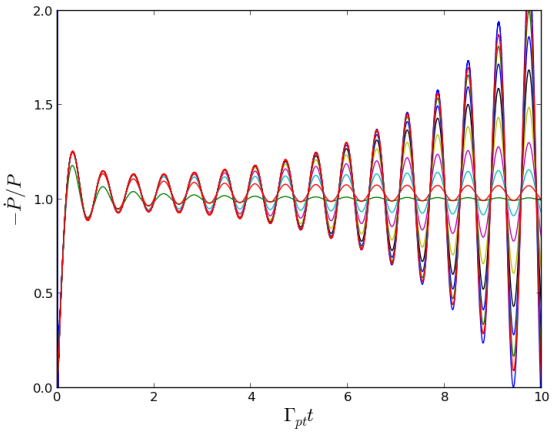


(d) Lorenzian W, $\Delta E = 2\hbar\Gamma$.

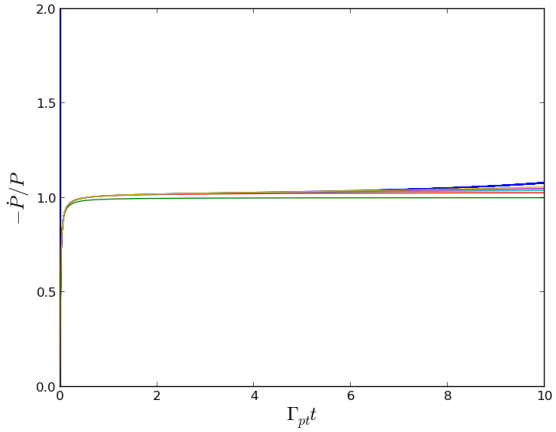
Figure 6.14: Instantaneous decay rate, comparison between exact result and Markovian approximations to various orders. The blue curve is the exact result. How the order varies among the remaining curves should be obvious. This figure shows systems where the memory kernel is exponentially bounded.



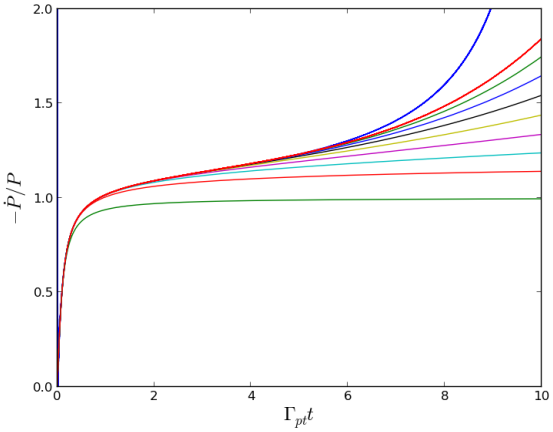
(a) Flat W, $\Delta E = 80\hbar\Gamma$.



(b) Flat W, $\Delta E = 10\hbar\Gamma$.



(c) Exponential W, $\Delta E = 80\hbar\Gamma$.



(d) Exponential W, $\Delta E = 10\hbar\Gamma$.

Figure 6.15: Instantaneous decay rate, comparison between exact result and Markovian approximations to various orders. The blue curve is the exact result. How the order varies among the remaining curves should be obvious. This figure shows systems where the memory kernel is not exponentially bounded.

and there is no reason to believe this does not happen after a sufficiently high order. One might argue that this slow convergence indicates that the Markovian expansion does not work to well in this case, but one should keep in mind that $\Delta E = 2\hbar\Gamma$ corresponds to very strong interactions for a method that is designed to work best in the weak interaction limit. Also, the 6. order curve does in fact not visibly separate from the exact one before well after two decay times.

In figure 6.15, where there is no asymptotic decay rate, the expansion curves does not converge as quickly as in 6.14. Here to however, they seem to approach the exact result and there is no reason to assume they will not converge after a sufficiently high order. Note for instance figure b, where each new order results in more rapidly increasing oscillations, approaching the exponential increment in the exact curve.

6.9 Summary of conclusions

6.9.1 Concerning the system

In the very simple model described in this chapter, the coupling to the environment really only causes two phenomenons of any interest. One: it causes incoherent transitions from the excited state $|e\rangle$ to the ground state $|g\rangle$, and two: it causes an alteration of the rate by which the phase difference between the two states changes. In some models (as will be exemplified in the next chapter) we have an additional phenomenon where the diagonal and non-diagonal elements of the state operator changes over different time scales. As can be seen from equation 6.25 this is not the case in this simple model. This is due to the extremely simple form of the Hamiltonian 6.1.

In the limit of weak interactions, the development of the phase difference between the states can be described simply by a shift in energy of the excited state: a Lamb shift. We see however from figure 6.6 that in general the story is more complicated than this: The rate of the phase difference is really a function of time that oscillates around some average. We can approximate this by letting the rate be constant and equal to the average. This would then be the Lamb shift, and we expect the approximation to get better as the interaction strength decreases.

Figure 6.6 is really the only place where the question concerning the development of phases is studied. In the entire rest of the chapter we are concerned with the first phenomenon, and we study the development of the probabilities for being in state $|e\rangle$ or $|g\rangle$. This is really a more interesting phenomenon, as it is connected to the decay of an energetic state as explained in the introduction to the chapter. The conventional assumption is that this decay is exponential, that is it is expected that the probability for being in the $|e\rangle$ state has the simple form 6.17.

One of the conclusions of this chapter is that this is in fact only the case when we have separation of the two time scales $\tau_1 = \hbar/\Delta E$ and $\tau_2 = 1/W(0)$: Exponential decay is an approximation that works exceedingly well when $\tau_1 \ll \tau_2$, but when this is not the case the decay may take on a form that is anything but exponential. This is exemplified for instance in figure 6.13, where the blue curve shows the exact development of $P_e(t)$ in cases where the interaction strength $W(0)$ is comparable to the energy range ΔE. Also, even in the cases where we do have time scale separation, there are deviations from the exponential development at sufficiently short time scales: when $t \ll \tau_1$ the probability falls of quadratically.

We have however also found that it seems the decay may be asymptotically exponential without time scale separation. More precisely this seems to be the case when the Fourier transform of the W function is exponentially bounded. In fact the asymptotic form seems to be completely unconnected to the question of time scale separation: When this Fourier transform is not exponentially bounded, the development deviates from exponential decay also in the weakly interacting cases at sufficiently large times. See for instance the figures 6.9 and 6.10 and the discussion in section 6.6.3. This was found to be in agreement with the references [13] and [6].

An entirely different question than the one concerning exponential decay, is whether the decay is Markovian. That is, whether it can be described by some Markovian generator. If this generator is time independent, then the decay must indeed be exponential. In general however, the generator may depend

on time and can result in completely different behavior. In fact, the only case in the chapter where we have demonstrated with certainty that the decay can not be described in a Markovian fashion, is in figure 6.13(e). Here the development is Markovian in some short interval after initialization, and the suddenly changes its behavior in a way that the Markovian expansions can not reproduce.

As long as we assume the environmental oscillators to form a continuum, it seems that all the other cases in the chapter have Markovian descriptions in the ranges where they are studied. To the question of whether this model have any non-Markovian characteristics we must therefore answer that this is highly parameter sensitive: Behavior that is manifestly non-Markovian does not seem to appear unless we have interactions that are very strong. In figure 6.13(e) for instance we have $\hbar\Gamma = 2\pi W(0) = 2\Delta E$. And even then it takes some time before the non-Markovian character appears. That behavior which is non-Markovian in this strict meaning of the word is something that is difficult to achieve is in well agreement with the discussion in part 1 (See for instance section 4.2).

Finally, we also discussed the effects of having an environment of finite size: When the environmental bath contains only a finite number of oscillators, we no longer have a decay in the same sense. That is, the probability of remaining in the excited state does not go to 0 as $t \to \infty$. Instead it decreases in some initial time interval but then suddenly changes its character and starts growing again. These sudden changes repeat themselves with a fixed period, so that the state does not have any meaningful limit (See figure 6.3). We saw that this behavior could be understood as a consequence of the fact that the memory kernel of such finite baths are periodic.

6.9.2 Concerning the methods

In this chapter we have used several methods to analyze the behavior of this very simple system: This includes exact diagonalization, several different perturbation expansions and an exact memory equation for the probability amplitude $c(t)$. I will now briefly discuss the consistency of these methods among each other, the parameter ranges in which they are useful and which of them are useful also for more complicated models.

The standard perturbation theory expansion, which is here only taken to the first order is supposed to work for short times t. And indeed, it is in well agreement with the other methods in this range while it deviates strongly from anything sensible at larger times. This is not unexpected. The Redfield equation, which is similarly the first order expansion of the Markovian generator described in section 5.4 works well for arbitrarily large times t, but also as expected only when the time scale separation criterion $\tau_1 \ll \tau_2$ is satisfied. See for instance figure 6.4.

We would expect that the performance of the Redfield equation can be improved upon by going to higher order in the Markovian generator, and in section6.8 we saw this to indeed be the case: By going to a sufficiently high order it seems we can make the solutions converge to the exact result even when the interaction strength is comparable to the energy range ΔE. Or that is, when τ_1 is comparable to τ_2. In fact, the only limitation of this Markovian expansion seems to be that we might be dealing with a system that is truly non-Markovian, as in figure 6.13(e). And even then the Markovian expansion works just fine in the interval between 0 and 1.4.

As long as we are not dealing with a manifestly non-Markovian system it seems that to expand the Markovian generator like this is the best approach. As long as the timescale separation criterion is satisfied and enormous accuracy is not required, it is even quite safe to limit the expansion to the first order corresponding to the Redfield/Lindblad equation. If we are however dealing with a system that is manifestly non-Markovian, and we in addition wish solutions that apply beyond the short time interval where the development remains Markovian, then we must use other methods.

One possible such method is exact diagonalization. In the particular model studied in this chapter exact diagonalization works very well. This is certainly the case for finite environments, and even with continuous ones the diagonalization results form good approximations in the interval $[0, 2\pi/\delta\omega]$ (See again figure 6.3). The main reason diagonalization works so well here is however the extreme simplicity of the model. In particular the numerical requirements are dramatically reduced by working in the closed subspace described in the introduction to the chapter.

If we are dealing with a system that is more complicated than a two-level system or wish to use more realistic models of the environment and the interactions with this, then we must expect exact diagonalization to be very numerically demanding if any meaningful accuracy is attempted. In addition to this, in more general models it might be much more difficult to extract the relevant information about the reduced system S from the solution of the total system T. This will be exemplified in the next chapter. The diagonalization method is therefore not a a method that generalizes in a good way to more complicated models. All though, as will demonstrated in the next section, other related exact methods can sometimes be applied.

The best method for treating non-Markovian systems seems in fact to be the use of a memory equation. Particularly this is the case when we have access to an exact memory kernel. This turned out to be a very powerful approach, as it provided a believable treatment of a lot of different interesting questions: It gave us both a way to study the asymptotic development of the system, and a quantitative understanding of the consequences of a finite size environment. As long as the kernel only depends on the difference $t - t'$ it is not even particularly demanding to solve the equation numerically.

The only problem with this method is that we in general do not have access to an exact kernel. In generalizing the method to more complicated systems we must therefore make do with an expansion of the Nakajima Zwanzieg kernel as described in section 5.2. The results in section 6.7 however seem to indicate that the solution given such expansions converge nicely towards the exact results (See figure 6.12). A problem with that expansion is however that the process of calculating the contributions of different orders is very laborious, even in the case of such a very simple model as this one. This problem can be assumed to be even larger for the Markovian expansion of form 5.36 to 5.40, as these expressions are clearly more complicated than 5.14. If we wish to take either of these expansions to a particularly high order, some computer automation is clearly needed.

Chapter 7

The Open Harmonic oscillator

7.1 Description of the model

The next model we shall consider will also be a simple one, although not as simple as the previous: It is an open quantum harmonic oscillator. That is, it is a standard quantum harmonic oscillator of the type described in section 2.3.2, coupled to an environment. This environment will again be modeled in an as simple a way as possible: namely as a bath consisting of more oscillators. Also, the interaction between the oscillators will be taken to be of a type that conserves the total excitation number of the system. That is, we again make the rotating wave approximation. This approximation is common in quantum optics[2], which is why I will sometimes refer to this model as the quantum optical harmonic oscillator.

The open harmonic oscillator provides a simplified description of quite a lot of different systems. It could represent a mechanical oscillator, such as the vibrations of a macroscopic spring or a chemical bond, t could represent an optical mode, such as for instance in a laser or some other application of optical cavities and it could represent a mode in some other bosonic field, such as a field of pions or other nuclear bosons, and it could provide a highly simplified model of the energy levels of an atom or molecule.

In applying the model to one of these systems, one would however have to keep in mind that the interactions between these and their environment are in reality not number conserving: the rotating wave approximation is only a good approximation as long as the interaction strength is weak in comparison to the energy scale of the system. In this case this scale would be $\hbar\omega$, where ω is the frequency of the oscillator. This would typically not be the case with a mechanical oscillator, but if we are dealing with a bosonic mode or some atomic system there is usually several orders of magnitude between these quantities.

Let us go into some more detail in describing the model. We assume that our system S is a harmonic oscillator of frequency ω, and that it is coupled to an environment E which also consists of harmonic oscillators. The individual oscillators of the environment we shall index with $i = 1 \cdots N$, N being the number of oscillators in E and possibly ∞. The frequencies of the environmental oscillators we denote ω_i, and the number, annihilation and creation operators we denote n_i, a_i and $a_i^\dagger$. The number, annihilation and creation operators of S we denote simply n, a and $a^\dagger$.

With these definitions we are ready to write up the Hamiltonian of the total system $T = S \cup E$, which is

$$H_T = H_S + H_E + H_{SE} = \hbar\omega n + \sum_i (\hbar\omega_i n_i + w_i a^\dagger a_i + w_i^\star a a_i^\dagger), \tag{7.1}$$

where we have introduced the parameters w_i, controlling the interaction between S and oscillator i. The Hamiltonian 7.1 can be written in a more compact form if we make a few definitions: We define a vector

$\boldsymbol{a}$ having a as its 0'th component, and a_i as its i'th component. We also define a matrix W as

$$W = \begin{pmatrix} \hbar\omega & w_1 & w_2 & \cdots & w_N \\ w_1^\star & \hbar\omega_1 & 0 & \cdots & 0 \\ w_2^\star & 0 & \hbar\omega_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ w_N^\star & 0 & 0 & \cdots & \hbar\omega_N \end{pmatrix}. \tag{7.2}$$

With these definitions 7.1 can be expressed simply as

$$H_T = \boldsymbol{a}^\dagger W \boldsymbol{a}. \tag{7.3}$$

In this entire section we shall assume that we have factorizing initial conditions: $\rho_T(0) = \rho(0) \otimes \rho_E(0)$. The initial state $\rho_E(0)$ of the environment we will assume to be thermal. That is we assume $\rho_E(0) = \frac{1}{Z} e^{-\beta H_E} = \prod_i (1 - e^{-\beta\omega_i}) e^{-\beta\hbar\omega_i n_i}$. On the other hand, we assume that the oscillator S in principle can be in any state. Although, we will of course choose a few specific ones as examples. In particular these will be simple superpositions of energy-eigenstates and coherent states.

7.2 Outline of the chapter

We will begin the analysis of this chapter by applying the Redfield equation. This of course assumes as before that we are in the limit of weak interactions. The Redfield equation will be applied in section 7.3. In section 7.3.1 we will first derive this equation for the model 7.1 by explicitly calculating the integral in 4.30. This will be done under the assumption that the environment is in a thermal state.

In sections 7.3.2 and 7.3.3 we then temporarily specialize to temperature 0, that is an environment in the vacuum state, and we analyze the development of the system first in the coherent state representation (in section 7.3.2), and then in the energy/number representation (in section 7.3.3). We will in both sections first analyze what happens to a single state in the basis, and then try to say something about what happens to superpositions of these states.

In section 7.3.4 we depart from the $T = 0$ specialization, and move back to general thermal environments. These will only be analyzed in the coherent state basis. This analysis will be performed by solving the Redfield equation for the 'matrix elements' $\rho(u, v) = \langle u| \rho |v\rangle$, where $|u\rangle$ and $|v\rangle$ are coherent states. In analyzing the solution we will again first look at what happens to a single coherent state, and then try to see what happens to superpositions.

After this we are done with the study of the weak interaction limit, and we will proceed with solving the system exactly. This will be done in section 7.4. This solution will be found by decoupling the oscillators through a simple diagonalization. If it is again assumed that the environment starts out in the vacuum state, then this solution is easily reduced to a description of the system S alone. This is done in section 7.4.1. We will see that the solutions take on the same form as in the weak interaction limit, but that certain parameters behave differently.

If however the environment starts out in a general thermal state, then the reduced description of the system S is found only through an extensive amount of work. In section 7.4.2 this is done by integrating over all possible environmental configurations, expressed in the coherent state representation. Once again we find that the solutions have the same form as in the weak interaction limit, but that again certain parameters of the solution behave differently. In particular, the heating of the oscillator takes on a more complicated form than in the Redfield result.

I mentioned that one of the things we will study is the general consequences of having superpositions of coherent or energy basis-states. The most important such consequence is that of decoherence. This is a new phenomenon which was not encountered in the previous model. Roughly speaking decoherence means that superpositions of states from certain special bases will quickly approach a classical mix of these states. This has the consequence that over long time scales the system behaves to a large degree classically. In the final section, section 7.4.3 we will observe what consequences an environment of finite size has on decoherence. In particular we will observe how these consequences depend on temperature.

7.3 Redfield/Lindblad equation

7.3.1 derivation

As mentioned we first analyze the model in the weak interaction limit. That is, in the limit that the interaction coefficients w_i are small when compared with the relevant energy range of the environment. This will allow us to apply the Redfield equation 4.30, and thus perform a simple Markovian analysis. In order to do this, we must obviously first explicitly express the Redfield equation in terms of the parameters of our model. In particular, this means we must calculate the operator $\mathrm{Tr}_E[H_{SE}(t),[H_{SE}(t-t'),\rho_S(t)\otimes\rho_E(0)]]$. The operator $H_{SE}(t)$ is the interaction part of the Hamiltonian, expressed in the interaction picture. In our case this is simply

$$H_{SE}(t)=\sum_i (w_i a^\dagger(t)a_i(t)+w_i^\star a(t)a_i^\dagger(t)), \tag{7.4}$$

where $a(t)=a\cdot e^{-i\omega t}$, $a^\dagger(t)=a^\dagger\cdot e^{i\omega t}$ and the environmental operators are given by completely analogous expressions.

In the following calculation we will find it useful to know the expectation values $\langle a_i\rangle$ and $\langle N_i\rangle$ in a thermal state, so we will begin by calculating these. By employing 2.39 this is done as follows:

$$\langle a_i\rangle=\mathrm{Tr}a_i(1-e^{-\beta\hbar\omega_i})e^{-\beta\omega_i n_i}=(1-e^{-\beta\hbar\omega_i})\sum_n e^{-\beta\hbar\omega_i n}\langle n|\,a_i\,|n\rangle=0, \tag{7.5}$$

$$\begin{aligned}\langle n_i\rangle&=\mathrm{Tr}n_i(1-e^{-\beta\hbar\omega_i})e^{-\beta\omega_i n_i}=(1-e^{-\beta\hbar\omega_i})\sum_n e^{-\beta\hbar\omega_i n}\langle n|\,N_i\,|n\rangle\\&=(1-e^{-\beta\hbar\omega_i})\sum_n ne^{-\beta\hbar\omega_i n}=\frac{(1-e^{-\beta\hbar\omega_i})e^{-\beta\hbar\omega_i}}{(1-e^{-\beta\hbar\omega_i})^2}=\frac{1}{e^{\beta\hbar\omega_i}-1}.\end{aligned} \tag{7.6}$$

By a completely similar calculation we find that $\langle a_i^\dagger\rangle$, $\langle a_i^2\rangle$ and $\langle a_i^{2\dagger}\rangle$ will be zero just like $\langle a_i\rangle$. Also, obviously $\langle a_i a_i^\dagger\rangle=\langle a_i^\dagger a_i+1\rangle=\langle n_i\rangle+1$.

Knowing this, it is easy to find expressions for the more general expectation values $\langle a_i a_j\rangle$, $\langle a_i^\dagger a_j\rangle$, $\langle a_i a_j^\dagger\rangle$ and $\langle a_i^\dagger a_j^\dagger\rangle$. First, if i and j are not equal the expectation values factorizes. For instance $\langle a_i a_j\rangle=\langle a_i\rangle\langle a_j\rangle=0$. It is easily seen that all of these expectation values will be zero like this. On the other hand, if i and j are equal, then the expressions coincide with one of the expectation values calculated above. We thus find that $\langle a_i a_j\rangle$ and $\langle a_i^\dagger a_j^\dagger\rangle$ are always zero, whereas $\langle a_i^\dagger a_j\rangle=\langle n_i\rangle\delta_{ij}$ and $\langle a_i a_j^\dagger\rangle=(\langle n_i\rangle+1)\delta_{ij}$.

These findings will be used in the calculation of a set of partial traces, all of which will be in the form $\mathrm{Tr}_E[A\otimes B,[C\otimes D,\rho\otimes\rho_E]]$. To simplify the calculations, we first find a general expression for partial traces in this form.

$$\begin{aligned}\mathrm{Tr}_E[A\otimes B,[C\otimes D,\rho\otimes\rho_E]]=&\mathrm{Tr}_E(A\otimes B\,C\otimes D\,\rho\otimes\rho_E-A\otimes B\,\rho\otimes\rho_E\,C\otimes D\\&-C\otimes D\,\rho\otimes\rho_E\,A\otimes B+\rho\otimes\rho_E\,C\otimes D\,A\otimes B)\\=&AC\rho\,\mathrm{Tr}\,BD\rho_E-A\rho C\,\mathrm{Tr}\,B\rho_E D-C\rho A\,\mathrm{Tr}\,D\rho_E B\\&+\rho CA\,\mathrm{Tr}\,\rho_E DB\\=&AC\rho\,\langle BD\rangle-A\rho C\langle DB\rangle-C\rho A\,\langle BD\rangle+\rho CA\,\langle DB\rangle\end{aligned} \tag{7.7}$$

With this, it is now easy to calculate

$$\mathrm{Tr}_E[a^\dagger(t_1)a_i(t_1),[a^\dagger(t_2)a_j(t_2),\rho\otimes\rho_E]] =$$

$$e^{i\omega(t_1+t_2)-i\omega_i(t_1+t_2)}(a^\dagger a^\dagger\rho\langle a_i a_j\rangle - a^\dagger\rho a^\dagger\langle a_i a_j\rangle - a^\dagger\rho a^\dagger\langle a_j a_i\rangle + \rho a^\dagger a^\dagger\langle a_j a_i\rangle) = 0, \quad (7.8)$$

$$\mathrm{Tr}_E[a(t_1)a_i^\dagger(t_1),[a^\dagger(t_2)a_j(t_2),\rho_S\otimes\rho_E]] =$$

$$e^{i\omega(t_2-t_1)+i\omega_i(t_1-t_2)}(aa^\dagger\rho\langle a_i^\dagger a_j\rangle - a^\dagger\rho a\langle a_i^\dagger a_j\rangle) - a\rho a^\dagger\langle a_j a_i^\dagger\rangle + \rho_S a^\dagger a\langle a_j a_i^\dagger\rangle) =$$

$$(\langle n_i\rangle(aa^\dagger\rho - a^\dagger\rho a) + (\langle n_i\rangle+1)(\rho a^\dagger a - a\rho a^\dagger))e^{i\omega(t_2-t_1)+i\omega_i(t_1-t_2)}\delta_{ij}, \quad (7.9)$$

and by simply taking the Hermitian conjugates of these formulas we also find

$$\mathrm{Tr}_E[a(t_1)a_i^\dagger(t_1),[a(t_2)a_j^\dagger(t_2),\rho\otimes\rho_E]] = 0, \quad (7.10)$$

$$\mathrm{Tr}_E[a^\dagger(t_1)a_i(t_1),[a(t_2)a_j^\dagger(t_2),\rho_S\otimes\rho_E]] =$$

$$(\langle n_i\rangle(\rho aa^\dagger - a^\dagger\rho a) + (\langle n_i\rangle+1)(a^\dagger a\rho - a\rho a^\dagger))e^{i\omega(t_1-t_2)+i\omega_i(t_2-t_1)}\delta_{ij}. \quad (7.11)$$

We are now ready to calculate the sought operator $\mathrm{Tr}_E[H_{SE}(t),[H_{SE}(t-t'),\rho_S(t)\otimes\rho_E(0)]]$. By applying the formulas 7.8 to 7.11 we finally find

$$\mathrm{Tr}_E[H_{SE}(t),[H_{SE}(t-t'),\rho(t)\otimes\rho_E]] =$$

$$\mathrm{Tr}_E\left[\sum_i(w_i a^\dagger(t)a_i(t) + w_i^\star a(t)a_i^\dagger(t)),\left[\sum_i(w_i a^\dagger(t-t')a_i(t-t') + w_i^\star a(t-t')a_i^\dagger(t-t')),\rho(t)\otimes\rho_E\right]\right] =$$

$$\sum_{ij}\Big(w_i w_j[a^\dagger(t)a_i(t),[a^\dagger(t-t')a_j(t-t'),\rho(t)\otimes\rho_E]] + w_i^\star w_j[a(t)a_i^\dagger(t),[a^\dagger(t-t')a_j(t-t'),\rho(t)\otimes\rho_E]] +$$

$$w_i w_j^\star[a^\dagger(t)a_i(t),[a(t-t')a_j^\dagger(t-t'),\rho(t)\otimes\rho_E]] + w_i^\star w_j^\star[a^\dagger(t)a_i^\dagger(t),[a^\dagger(t-t')a_j^\dagger(t-t'),\rho(t)\otimes\rho_E]]\Big) =$$

$$\sum_i|w_i|^2\Big(e^{-i(\omega-\omega_i)t'}(\langle n_i\rangle(aa^\dagger\rho - a^\dagger\rho a) + (\langle n_i\rangle+1)(\rho a^\dagger a - a\rho a^\dagger)) +$$

$$e^{i(\omega-\omega_i)t'}(\langle n_i\rangle(\rho aa^\dagger - a^\dagger\rho a) + (\langle n_i\rangle+1)(a^\dagger a\rho - a\rho a^\dagger))\Big) =$$

$$\sum_i|w_i|^2\Big(\cos(\omega-\omega_i)t'\cdot(\langle n_i\rangle(\{aa^\dagger,\rho\} - 2a^\dagger\rho a) + (\langle n_i\rangle+1)(\{a^\dagger a,\rho\} - 2a\rho a^\dagger))$$

$$+ i\sin(\omega-\omega_i)t'\cdot(\langle n_i\rangle[\rho,aa^\dagger] + (\langle n_i\rangle+1)[a^\dagger a,\rho])\Big) =$$

$$\int d\Omega\, W\left((n(\{aa^\dagger,\rho\} - 2a^\dagger\rho a) + (n+1)(\{a^\dagger a,\rho\} - 2a\rho a^\dagger))\cos(\omega-\Omega)t' + i[a^\dagger a,\rho]\sin(\omega-\Omega)t'\right), \quad (7.12)$$

where we in the last line have defined the functions $W(\Omega) = \sum_i|w_i|^2\delta(\Omega-\omega_i)$ and $n(\beta,\Omega) = 1/(e^{\beta\hbar\Omega}-1)$.

In order for the Redfield equation 4.30 to make sense, we must have a continuum of frequencies in the environment. Otherwise the quantity calculated above would be periodic, and to integrate over the entire

past would be meaningless. It is however easy to take the continuum limit of 7.12, since all that happens is that the W function becomes continuous and finite. When this is the case we may insert 7.12 in 4.30 to get

$$\begin{aligned}\dot{\rho} =& -\frac{1}{\hbar^2}\int_0^\infty \mathrm{Tr}_E[H_{SE}(t),[H_{SE}(t-t'),\rho(t)\otimes\rho_E(0)]]dt' \\ =&(2a^\dagger\rho a - \{aa^\dagger,\rho\})\frac{1}{\hbar^2}\int_0^\infty dt\int d\Omega W(\Omega)n(\beta,\Omega)\cos(\omega-\Omega)t \\ &+(2a\rho a^\dagger - \{a^\dagger a,\rho\})\frac{1}{\hbar^2}\int_0^\infty dt\int d\Omega W(\Omega)(n(\beta,\Omega)+1)\cos(\omega-\Omega)t \\ &-[a^\dagger a,\rho]\frac{i}{\hbar^2}\int_0^\infty dt\int d\Omega W(\Omega)\sin(\omega-\Omega)t. \end{aligned} \tag{7.13}$$

The integrals in this expression can be evaluated by recognizing that they are in fact nested Fourier integrals: We define the Fourier transform $\mathcal{F}$ and its inverse $\mathcal{F}^{-1}$ as

$$(\mathcal{F}f)(\Omega) = \int_{-\infty}^{\infty} f(t)e^{-i\Omega t}dt, \tag{7.14}$$

$$\left(\mathcal{F}^{-1}g\right)(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} g(\Omega)e^{i\Omega t}d\Omega. \tag{7.15}$$

This allows us to write

$$\begin{aligned}&\int_0^\infty dt\int d\Omega W(\Omega)n(\beta,\Omega)\cos(\omega-\Omega)t = \frac{1}{2}\int_0^\infty dt\int d\Omega W(\Omega+\omega)n(\beta,\Omega+\omega)(e^{i\Omega t}+e^{-i\Omega t}) \\ &=\frac{1}{2}\int_{-\infty}^\infty dt\int d\Omega W(\Omega+\omega)n(\beta,\Omega+\omega)e^{-i\Omega t} = \frac{1}{2}\int_{-\infty}^\infty dt\mathcal{F}\,W(\Omega+\omega)n(\beta,\Omega+\omega) \\ &=\frac{1}{2}2\pi\left(\mathcal{F}^{-1}\mathcal{F}\,W(\Omega+\omega)n(\beta,\Omega+\omega)\right)\big|_{\Omega=0} = \pi W(\omega)n(\beta,\omega). \end{aligned} \tag{7.16}$$

Obviously, in precisely the same way we also find

$$\int_0^\infty dt\int d\Omega W(\Omega)(n(\beta,\Omega)+1)\cos(\omega-\Omega)t = \pi W(\omega)(n(\beta,\omega)+1), \tag{7.17}$$

while the last integral can be simplified as

$$\begin{aligned}&\int_0^\infty dt\int d\Omega W(\Omega)\sin(\omega-\Omega)t = \frac{1}{2i}\int_0^\infty dt\int d\Omega W(\Omega+\omega)(e^{i\Omega t}-e^{-i\Omega t}) \\ &=-\frac{1}{2i}\int_{-\infty}^\infty dt\,\mathrm{sgn}(t)\int d\Omega W(\Omega+\omega)e^{-i\Omega t} = -\frac{1}{2i}\int_{-\infty}^\infty dt\,\mathrm{sgn}(t)\mathcal{F}\,W(\Omega+\omega) \\ &=-\frac{1}{2i}2\pi\left(\mathcal{F}^{-1}\mathrm{sgn}(t)\mathcal{F}W(\Omega+\omega)\right)\big|_{\Omega=0} = \pi i\left(\mathcal{F}^{-1}\mathrm{sgn}(t)*W(\Omega+\omega)\right)\big|_{\Omega=0} \\ &=\pi i\int_{-\infty}^\infty\frac{1}{-i\pi\Omega}W(\Omega+\omega)d\Omega = -\int\frac{d\Omega}{\Omega}W(\Omega+\omega). \end{aligned} \tag{7.18}$$

Here we have used the facts that the inverse Fourier transform of a product is the convolution of the individual transforms, and that the inverse Fourier transform of the sign function $\mathrm{sgn}(t) = t/|t|$ is $1/(-i\pi\Omega)$.

If we now make the definitions $\gamma = 2\pi/\hbar^2\cdot W(\omega)$, $n = n(\beta,\omega)$ and $\delta = -\frac{1}{\hbar^2}\int\frac{d\Omega}{\Omega}W(\Omega+\omega)$, then we see that 7.13 can be expressed as

$$\dot{\rho} = -i\delta[a^\dagger a,\rho] + \gamma(n+1)(a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a,\rho_S\}) + \gamma n(a^\dagger\rho_S a - \frac{1}{2}\{aa^\dagger,\rho_S\}). \tag{7.19}$$

Equation 7.19 is the Redfield equation of the quantum optical oscillator. Being a Redfield equation, it is expressed in the interaction picture. It is however easy to transform it to a corresponding equation in the Schrödinger picture: If ρ_S signifies the state operator in the Schrödinger picture, ρ_I signifies the same operator in the interaction picture and $U_0 = e^{-H_S t/\hbar}$ is the time development operator of the noninteracting Hamiltonian H_S, then generally we have

$$\dot{\rho}_S = \frac{d}{dt} U_0 \rho_I U_0^\dagger = \frac{d}{dt} U_0 \dot{\rho}_I U_0^\dagger - \frac{i}{\hbar}[H_S, \rho_S]. \tag{7.20}$$

In our case we thus simply get

$$\dot{\rho}_S = -i\omega'[a^\dagger a, \rho_S] + \gamma_1(a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a, \rho_S\}) + \gamma_2(a^\dagger \rho_S a - \frac{1}{2}\{aa^\dagger, \rho_S\}), \tag{7.21}$$

where we have made the further definitions $\omega' = \omega + \delta$, $\gamma_1 = \gamma(n+1)$ and $\gamma_2 = \gamma n$. We see that this equation is in Lindblad form.

7.3.2 Vacuum environment

The open harmonic oscillator will have the simplest behavior in the case where we in addition to making a Markovian approximation also assume that the environment has temperature zero. That is, we assume that it is in the vacuum state. In this case $n = n(\beta, \omega) = n(\infty, \omega) = 0$, which means that 7.21 simplifies to

$$\dot{\rho} = -\omega'[a^\dagger a, \rho] + \gamma(a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}), \tag{7.22}$$

This equation has particularly simple solutions in terms of coherent states. In order to examine what happens to superpositions of several coherent states, we will solve the equation for the operators $\mathcal{G}_t \left|z\right\rangle \left\langle w\right|$, with $\left|z\right\rangle$ and $\left|w\right\rangle$ being coherent states and $\mathcal{G}_t$ being the super operator defined by $\mathcal{G}_t \rho(0) = \rho(t)$. As long as we know the values of these operators, it is easy to find the development of any superposition of coherent states by the formula

$$\mathcal{G}_t \left(\sum_i c_i \left|z_i\right\rangle \cdot \sum_i c_i^\star \left\langle z_i\right| \right) = \sum_{ij} c_i c_j^\star \mathcal{G}_t(\left|z_i\right\rangle \left\langle z_j\right|). \tag{7.23}$$

In order to calculate $\mathcal{G}_t \left|z\right\rangle \left\langle w\right|$, we simply solve 7.22 with the initial value $\left|z\right\rangle \left\langle w\right|$. It turns out that the development is expressable as $\left|z(t)\right\rangle \left\langle w(t)\right| f(t)$, with $z(t)$, $w(t)$ and $f(t)$ complex functions. To find these functions we will simply insert this ansatz into 7.22. In order to do that however, we must find an expression for $\frac{d}{dt}\left|z(t)\right\rangle$. By employing the definitions 2.43 and 2.42 we can do this in the following way:

$$\begin{aligned}
\frac{d}{dz}\left|z\right\rangle &= \frac{d}{dz} D(z)\left|0\right\rangle = \frac{d}{dz} e^{-\frac{1}{2}|z|^2} e^{za^\dagger} e^{-z^\star a}\left|0\right\rangle \\
&= -\frac{1}{2} z^\star e^{-\frac{1}{2}|z|^2} e^{za^\dagger} e^{-z^\dagger a}\left|0\right\rangle + e^{-\frac{1}{2}|z|^2} a^\dagger e^{za^\dagger} e^{-z^\dagger a}\left|0\right\rangle = (-\frac{1}{2} z^\star + a^\dagger)\left|z\right\rangle, \qquad (7.24) \\
\frac{d}{dz^\star}\left|z\right\rangle &= \frac{d}{dz^\star} D(z)\left|0\right\rangle = \frac{d}{dz^\star} e^{-\frac{1}{2}|z|^2} e^{za^\dagger} e^{-z^\star a}\left|0\right\rangle \\
&= -\frac{1}{2} z e^{-\frac{1}{2}|z|^2} e^{za^\dagger} e^{-z^\star a}\left|0\right\rangle - e^{-\frac{1}{2}|z|^2} e^{za^\dagger} e^{-z^\star a} a\left|0\right\rangle = -\frac{1}{2} z\left|z\right\rangle, \qquad (7.25) \\
\frac{d}{dt}\left|z\right\rangle &= \frac{dz}{dt}\frac{d}{dz}\left|z\right\rangle + \frac{dz^\star}{dt}\frac{d}{dz^\star}\left|z\right\rangle = (-\frac{1}{2} z^\star \dot{z} + \dot{z} a^\dagger - \frac{1}{2} z \dot{z}^\star)\left|z\right\rangle = (-\mathcal{R}e z^\star \dot{z} + \dot{z} a^\dagger)\left|z\right\rangle. \qquad (7.26)
\end{aligned}$$

Note that we here regard z and $z^\star$ as being independent variables. With this we see that with our ansatz, 7.22 becomes

$$\begin{aligned} &- \mathcal{R}e(z^\star \dot{z} + w^\star \dot{w}) \left|z\right\rangle \left\langle w\right| f + \dot{z} a^\dagger \left|z\right\rangle \left\langle w\right| f + \dot{w}^\star \left|z\right\rangle \left\langle w\right| af + \left|z\right\rangle \left\langle w\right| \dot{f} \\ = &- i\omega' a_\dagger a \left|z\right\rangle \left\langle w\right| f + i\omega' \left|z\right\rangle \left\langle w\right| a_\dagger a f + \frac{\gamma f}{2}(2a \left|z\right\rangle \left\langle w\right| a^\dagger - a^\dagger a \left|z\right\rangle \left\langle w\right| - \left|z\right\rangle \left\langle w\right| a^\dagger a). \end{aligned} \tag{7.27}$$

By collecting coefficients that stand in front of the three different operators $\left|z\right\rangle \left\langle w\right|$, $a^\dagger \left|z\right\rangle \left\langle w\right|$ and $\left|z\right\rangle \left\langle w\right| a$, we see that this equation will be satisfied as long as the following three equations are:

$$-\mathcal{R}e(z^\star \dot{z} + w^\star \dot{w}) f + \dot{f} = \gamma f z w^\star, \tag{7.28}$$

$$\dot{z} f = -i\omega' z f - \frac{\gamma f}{2} z, \tag{7.29}$$

$$\dot{w}^\star f = i\omega' w^\star f - \frac{\gamma f}{2} w^\star. \tag{7.30}$$

The two lower equations have the two obvious solutions $z(t) = ze^{-i\omega' t - \gamma t/2}$ and $w(t) = we^{-i\omega' t - \gamma t/2}$, which turns the top one into

$$\frac{\gamma}{2}(|z|^2 + |w|^2) e^{-\gamma t} f + \dot{f} = \gamma f z w^\star e^{-\gamma t}, \tag{7.31}$$

or alternatively $\dot{f} = -\frac{\gamma_1}{2}(|z|^2 - 2zw^\star + |w|^2) e^{-\gamma_1 t} \cdot f$. Since $f(0) = 1$, the solution of this equation can be expressed as

$$f(t) = \exp\left(-\frac{\gamma_1}{2} \int_0^t (|z|^2 - 2zw^\star + |w|^2) e^{-\gamma_1 t}\right) = \exp\left(-\frac{1}{2}(1 - e^{-\gamma_1 t}) d(w, z)\right). \tag{7.32}$$

Where we have now defined the function $d(w, z) = |w|^2 - 2w^\star z + |z|^2$, which will be extensively used in this chapter. Note that the real value of this function is $\mathcal{R}e\, d(w, z) = |w|^2 - 2\mathcal{R}e\, w^\star z + |z|^2 = |w - z|^2$.

In total then, our findings tells us that

$$\mathcal{G}_t \left|z\right\rangle \left\langle w\right| = \left|zr(t)\right\rangle \left\langle wr(t)\right| \exp\left(-\frac{1}{2}(1 - |r(t)|^2) d(w, z)\right), \text{ with} \tag{7.33}$$

$$r(t) = e^{-i\omega' t - \frac{\gamma}{2} t}. \tag{7.34}$$

In particular, if we put $z = w$ we get the time development of $\rho(t)$ assuming that it is initialized in a coherent state. In this case $f(t) = 1$, and we see that the oscillator remains in a pure, coherent state at all times. To be precise, at time t it is in the state $\left|zr(t)\right\rangle = \left|ze^{-i\omega' t - \gamma t/2}\right\rangle$. Obviously, in this model the development of a coherent state is very similar to the development we would have if the oscillator was not coupled to the environment. In that case we would instead have just $\left|\psi(t)\right\rangle = \left|ze^{-i\omega t}\right\rangle$. We see then, that the only difference between the two cases is the shape of the orbit that the coherent state index z follows in the complex plane. The coupling to the the environment has two effects on this orbit: Firstly, the frequency is shifted by an amount δ, and secondly, the oscillations are exponentially damped out over a timescale $\tau = 1/\gamma$, so that we now have a damped harmonic oscillator.

If we do not start out in a coherent state, there will be one additional effect: that of decoherence. Decoherence simply means that as the the state develops it will not remain pure. Instead it will develop into a mixed state. To investigate this phenomenon in the oscillator model, let us assume that we start out in a pure state that is a superposition of two different coherent states $\left|z\right\rangle$ and $\left|w\right\rangle$. For instance we could take this to be $\left|\psi\right\rangle = (\left|z\right\rangle + \left|w\right\rangle)/\sqrt{2(1 + \mathcal{R}e \left\langle z|w\right\rangle)}$. Note that $\left\langle z|w\right\rangle$ is not 0, so that the normalization factor is not simply $1/\sqrt{2}$. Since this is in any case just a constant coefficient we may ignore it for simplicity.

If we do this, the state operator is just $\rho(0) = (|z\rangle + |w\rangle)(\langle z| + \langle w|) = |z\rangle\langle z| + |w\rangle\langle z| + |z\rangle\langle w| + |w\rangle\langle w|$. According to the equations 7.23 and 7.33 this will develop into

$$\rho(t) = |zr(t)\rangle\langle zr(t)| + |wr(t)\rangle\langle wr(t)| + \exp\left(-\frac{1}{2}d(w,z)1 - |r(t)|^2)\right)(|zr(t)\rangle\langle wr(t)| + |wr(t)\rangle\langle zr(t)|). \tag{7.35}$$

If the exponential factor $f(t) = \exp\left(-\frac{1}{2}(1-|r(t)|^2)d(w,z)\right)$ is largely damped out, the state will essentially be $|zr(t)\rangle\langle zr(t)| + |wr(t)\rangle\langle wr(t)|$, which is a mixed state corresponding to an evenly weighted mix of the two pure states $|zr(t)\rangle$ and $|wr(t)\rangle$. It therefore makes sense to take the absolute value $|f(t)|$ of this factor to represent the remaining degree of coherence in the state.

This absolute value is $|f(t)| = e^{-\frac{1}{2}(1-|r(t)|^2)|z-w|^2}$, and we see that it depends on the decay controlling factor $r(t)$ as well as the distance $|z-w|$ between the coherent state indexes z and w in the complex plane. It is easily seen that $|f(t)|$ will be damped when t increases. It will limit towards the quantity $e^{-\frac{1}{2}|z-w|^2}$, which becomes exponentially smaller when the distance between z and w is increased. We should note that this limit is in fact the absolute value of the overlap between the states $|z\rangle$ and $|w\rangle$.

Another effect of increasing this distance is that the rate by which the damping occurs will grow. In fact this rate will be given by $\gamma_D = \frac{\gamma}{2}|z-w|^2$, which can be demonstrated by noting that for $t \ll 1/\gamma$ $|f(t)|$ can be approximated as $|f(t)| = e^{-\frac{1}{2}(1-e^{-\gamma t})|z-w|^2} \approx e^{-\frac{1}{2}(1-(1-\gamma t))|z-w|^2} = e^{-\frac{1}{2}\gamma|z-w|^2 t}$. To illustrate these effects, $|c(t)|$ is shown for a few different distances $|z-w|$ in figure 7.1.

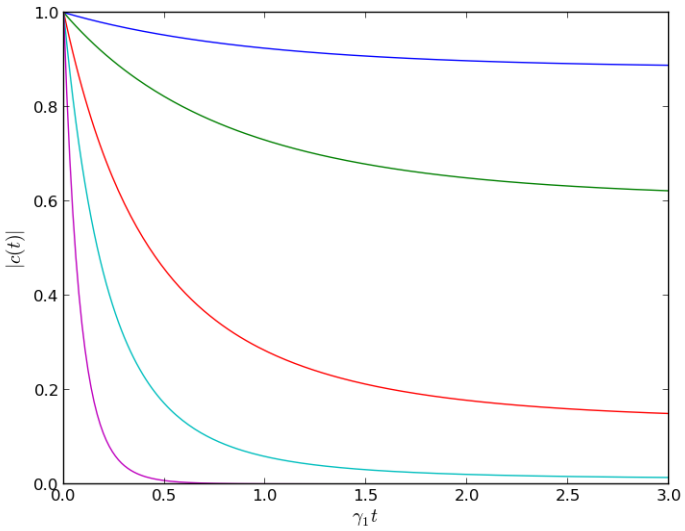


Figure 7.1: Plot of the quantity $|c(t)|$ against $\gamma_1 t$. $|z-w| = 0.5$, 1, 2, 3 and 5 are shown as the blue, green red, cyan and purple curves respectively. Note that the function falls of faster and stabilizes at lower values with increasing $|z-w|$.

7.3.3 Vacuum environment case expressed in energy basis

In the preceding we found an expression for the time development of the quantum optical harmonic oscillator expressed using coherent states. Another common basis used in analyzing harmonic oscillators is the energy, or n-basis. To analyze the development using this basis could be interesting also in this case. In this subsection we will therefore attempt to convert the formulas in the preceding to expressions in the n-basis. More precisely, we will calculate the operator $\mathcal{G}_t |n\rangle\langle m|$, where $|n\rangle$ and $|m\rangle$ are energy states.

This could also have been done by deriving a set of coupled differential equations for the matrix elements ρ_{nm} from 7.22, and then solving these. This is done in [2] and strictly speaking this is much

simpler than the method to be employed here. However, we shall find that the expression 7.33 actually generalizes to the exact solution of this model (although $r(t)$ no longer has the same simple form). Thus, if we instead derive the expressions for $\mathcal{G}_t \left|n\right\rangle \left\langle m\right|$ from this equation, then this result will also generalize to the exact solution. Therefore this is what I will do.

The first thing we should do then, is to express the initial value $\left|n\right\rangle \left\langle m\right|$ in terms of coherent states. This is easy.

$$\left|n\right\rangle \left\langle m\right| = \int \frac{d^2z}{\pi} \left|z\right\rangle \left\langle z\right| \left|n\right\rangle \left\langle m\right| \int \frac{d^2w}{\pi} \left|w\right\rangle \left\langle w\right| = \int \frac{d^2zd^2w}{\pi^2} \frac{z^{\star n}w^m}{\sqrt{n!m!}} e^{-\frac{1}{2}(|z|^2+|w|^2)} \left|z\right\rangle \left\langle w\right|, \tag{7.36}$$

where we have used the formula 2.46 for the overlap between a coherent state and an n-basis state.

Due to the linearity of the time development, the operator at time t can now be found easily from 7.35. This becomes

$$\mathcal{G}_t \left|n\right\rangle \left\langle m\right| = \int \frac{d^2zd^2w}{\pi^2} \frac{z^{\star n}w^m}{\sqrt{n!m!}} e^{-\frac{1}{2}(|z|^2+|w|^2)-\frac{1}{2}(1-|r|^2)d(w,z)} \left|zr\right\rangle \left\langle wr\right|. \tag{7.37}$$

We then proceed to calculate the quantity $\left\langle k\right| \left(\mathcal{G}_t \left|n\right\rangle \left\langle m\right|\right) \left|l\right\rangle$, with $\left|k\right\rangle$ and $\left|l\right\rangle$ new energy states:

$$\begin{aligned}
\left\langle k\right| \left(\mathcal{G}_t \left|n\right\rangle \left\langle m\right|\right) \left|l\right\rangle &= \int \frac{d^2zd^2w}{\pi^2} \frac{z^{\star n}w^m}{\sqrt{n!m!}} e^{-\frac{1}{2}(|z|^2+|w|^2)-\frac{1}{2}(1-|r|^2)d(w,z)} \left\langle k|zr\right\rangle \left\langle wr|l\right\rangle \\
&= \int \frac{d^2zd^2w}{\pi^2} \frac{z^{\star n}w^m(zr)^k(wr)^{\star l}}{\sqrt{n!m!k!l!}} \exp\left(-|z|^2 - |w|^2 + w^\star z(1-|r|^2)\right) \\
&= \frac{r^k r^{\star l}}{\sqrt{n!m!k!l!}} \int \frac{d^2w}{\pi} w^m w^{\star l} e^{-|w|^2} \int \frac{d^2z}{\pi} z^{\star n} z^k e^{-|z|^2} e^{(1-|r|^2)w^\star z} \\
&.
\end{aligned} \tag{7.38}$$

The inner integral above may be re-expressed as a complex curve integral in the following way:

$$\begin{aligned}
&\int \frac{d^2z}{\pi} z^{\star n} z^k e^{-|z|^2} e^{(1-|r|^2)w^\star z} = \int \frac{dRRd\theta}{\pi} |z|^{2n} z^{k-n} e^{-|z|^2} e^{(1-|r|^2)w^\star z} = \\
&\int \frac{dR}{\pi} R^{2n+1} e^{-R^2} \int d\theta z^{k-n} e^{(1-|r|^2)w^\star z} = \int \frac{dR}{\pi} R^{2n+1} e^{-R^2} \oint \frac{dz}{iz} z^{k-n} e^{(1-|r|^2)w^\star z},
\end{aligned} \tag{7.39}$$

where the curve integral is over a circle of radius R centered in the origin, and $d\theta = dz/iz$ since $dz = d(Re^{i\theta}) = id\theta Re^{i\theta} = id\theta z$.

The curve integral may be calculated using the complex analysis formula

$$f^{(n)}(w) = \frac{1}{2\pi i} \oint \frac{f(z)dz}{(z-w)^{n+1}}, \tag{7.40}$$

which tells us that

$$\oint \frac{dz}{iz} z^{k-n} e^{(1-|r|^2)w^\star z} = 2\pi i \frac{d^{n-k}}{dz^{n-k}} e^{(1-|r|^2)w^\star z}|_{z=0} = 2\pi i((1-|r|^2)w^\star)^{n-k} \tag{7.41}$$

if $n \geq k$, and otherwise zero. The R part of the integral is a simple Gaussian integral, and easy to calculate. In total, we find that

$$\int \frac{d^2z}{\pi} z^{\star n} z^k e^{-|z|^2} e^{(1-|r|^2)w^\star z} = \frac{n!}{(n-k)!}((1-|r|^2)w^\star)^{n-k}. \tag{7.42}$$

With this, 7.38 becomes

$$\langle k|\left(\mathcal{G}_t\ |n\rangle\langle m|\right)|l\rangle = \frac{r^k r^{\star l}}{\sqrt{n!m!k!l!}}\int\frac{d^2w}{\pi}\,w^m w^{\star l}e^{-|w|^2}\frac{n!}{(n-k)!}((1-|r|^2)w^\star)^{n-k}$$
$$= \frac{n!}{(n-k)!}\frac{r^k r^{\star l}(1-|r|^2)^{n-k}}{\sqrt{n!m!k!l!}}\left(\int\frac{d^2w}{\pi}\,|w|^{2m}e^{-|w|^2}w^{l+n-m-k}\right)^\star. \tag{7.43}$$

The integral in this expression may be calculated in precisely the same manner as above, and what we end up with is that it is $m!$ precisely when $l+n-m-k=0$, and otherwise zero. Finally then, we get

$$\langle k|\left(\mathcal{G}_t\ |n\rangle\langle m|\right)|l\rangle = \sqrt{\frac{m!n!}{k!l!}}\frac{(1-|r|^2)^{n-k}}{(n-k)!}r^k r^{\star l}\delta_{n-k,m-l} = \sqrt{\binom{n}{k}\binom{m}{l}}(1-|r|^2)^{n-k}r^k r^{\star l}\delta_{n-k,m-l}, \tag{7.44}$$

which applies when $n\geq k$ (and $m\geq l$). If this is not the case $\langle k|\left(\mathcal{G}_t\ |n\rangle\langle m|\right)|l\rangle = 0$.

Having now completed our calculations, we may turn to the analysis of our findings. The first thing we will examine is the time development of the oscillator given that it starts out in the pure state $|n\rangle\langle n|$. The matrix elements of the state operator may easily be found from 7.44. They are

$$\langle k|\,\rho(t)\,|l\rangle = \binom{n}{k}|r|^{2k}(1-|r|^2)^{n-k}\delta_{kl}, \tag{7.45}$$

when $n\geq k$, and otherwise zero.

The first thing we should note is that this $\rho(t)$ is diagonal in the n-basis. This means that if the oscillator starts out in an n-basis state, then it will remain a statistical mix of such states at all later times. This doesn't quite generalize the result from the previous subsection, where it was found that when starting out in a coherent state the oscillator remains a pure coherent state at all later times. It is however somewhat similar: Common in both of these cases is that the development can be described in purely classical terms.

In the case of coherent states we are dealing with a deterministic process, where at time t a particular coherent state is chosen deterministically from a coherent state at time 0. Whereas in the case of n-basis states we are obviously dealing with an indeterministic process, since we can not know with certainty what n state we will have at later times. The point is however that it is a classical indeterministic process, as all information is contained in the probabilities for being in different n-states. Both cases may thus be represented by a classical probability distribution, the only difference being that in the coherent state case the distribution would be a delta function.

Knowing then that the diagonal of $\rho(t)$ represents a simple classical probability distribution, we turn to examining the form of this distribution. It is easily seen that this is in fact a binomial distribution: $P(k)=\binom{n}{k}p^k(1-p)^{n-k}$, with $p=|r|^2$. This describes the probability of k positive results among n independent tests, where the probability of a positive result in a single test is $p=|r|^2$.

The interpretation of this result comes easiest if we assume that the oscillator describes a mode in a bosonic field, and that the damping represents decay of the bosonic particles. The oscillator being in the $|n\rangle$ state at time 0 then means that the mode initially contains n particles, and the $P(k)$ distribution is the probabilities of the mode containing k particles after time t. Let us assume that the probability of a single particle decaying is $1-|r|^2$. In the Markovian limit this would be $1-e^{-\gamma t}$, which would simply mean that the decay rate of the particles is γ. If the mode contains k particles, then this means that precisely k particles have not decayed. So let us then define not decaying as the positive result. This does indeed have probability $|r|^2$, which means the probability of k particles not decaying is described by precisely the binomial distribution above.

Having found an easily interpretable expression for the probability distribution, let us now turn to the question of decoherence. To examine this, we assume that the oscillator starts out in a superposition of several n-states, instead of just one as in the previous. The state operator will then have non-diagonal

matrix elements, and these are the ones that are of relevance to decoherence. In specific, let us assume the oscillator starts out in the state $\frac{|n\rangle+|m\rangle}{\sqrt{2}}$. This makes the state operator $\rho(0) = \frac{1}{2}(|n\rangle\langle n| + |n\rangle\langle m| + |m\rangle\langle n|+|m\rangle\langle m|)$, which means $\rho(t) = \frac{1}{2}(\mathcal{G}_t(|n\rangle\langle n|)+\mathcal{G}_t(|n\rangle\langle m|)+\mathcal{G}_t(|m\rangle\langle n|)+\mathcal{G}_t(|m\rangle\langle m|))$. As discussed the operators $\mathcal{G}_t(|n\rangle\langle n|)$ and $\mathcal{G}_t(|m\rangle\langle m|)$ will be purely diagonal. This means that the only non-diagonal contributions will come from $\mathcal{G}_t(|n\rangle\langle m|)$ and its Hermitian conjugate $\mathcal{G}_t(|m\rangle\langle n|)$.

Let us assume that $m > n$. Then since in order for 7.44 to be non-zero we must have $n = k$ and $m = l$, clearly we must have $l > k$ to get a non zero result in this expression. Thus it is clear that $\mathcal{G}_t(|n\rangle\langle m|)$ contributes only to the elements above the diagonal ($l > k$), while $\mathcal{G}_t(|m\rangle\langle n|)$ contributes only to the ones below it ($l < k$). This again means that in the case described, an element above the diagonal will be given by 7.44, and can be rewritten

$$\langle k|\rho(t)|l\rangle = \sqrt{\binom{n}{k}\binom{m}{l}}|r|^{2k}(1-|r|^2)^{n-k}r^{\star l-k}\delta_{n-k,m-l}. \tag{7.46}$$

We see that the only time dependent difference between these quantities and the binomial probability distribution of 7.45 is the factor $r^{\star l-k}$. Since $l > k$ above the diagonal this factor means that the non diagonal elements are damped relative to the probability distribution. The strength of the damping obviously grows with increasing $|k-l| = |n-m|$, and in the Redfield solution in particular it is given by $e^{-|k-l|\gamma t}$. This damping of non-diagonal matrix elements is illustrated in figure 7.2, where the state matrix is shown as a color plot at different times given the initial pure state $|\psi\rangle = (|25\rangle + |49\rangle)/\sqrt{2}$.

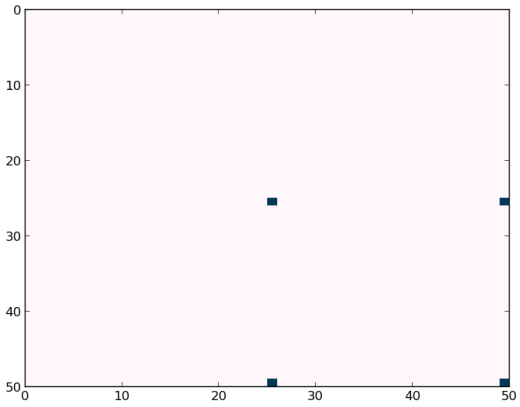
As a last remark we note that this damping of non diagonal elements means that a superposition of several n-states will approach a classical mix of such states as time progresses. This is a further generalization of our findings in the previous section, concerning superpositions of coherent states. In both cases we have found that not only will a classical mix of n-basis or coherent states remain a mix of such states, but a state which is not a such a mix will rapidly limit towards something which is reasonably close to one. This ads credibility to the idea that the oscillator may to good approximation be described in classical terms when using these bases.

7.3.4 Thermal environment

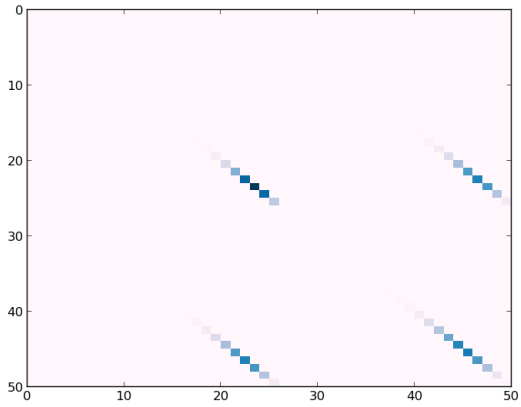
When the environment is not in the vacuum state, we must solve the full equation 7.21. We will then not be able to express the solution in such a simple form as 7.33, since no states will remain pure over the time development. Instead we shall solve the equation for the 'matrix elements' $\langle u|\rho|v\rangle$, with $|u\rangle$ and $|v\rangle$ coherent states. Let us denote these quantities $\rho(u,v)$. We would like to derive a differential equation for $\rho(u,v)$.

In order to do this we must first reexpress the action of a creation operator $a^\dagger$ on a coherent state in terms of derivatives. This can be done by comparison with 7.24. From that we see that in fact $a^\dagger|z\rangle = (\frac{1}{2}z^\star + \frac{\partial}{\partial z})|z\rangle$. In a very much similar calculation we would also find that $\langle z|a = (\frac{1}{2}z + \frac{\partial}{\partial z^\star})\langle z|$. This makes us able to now calculate

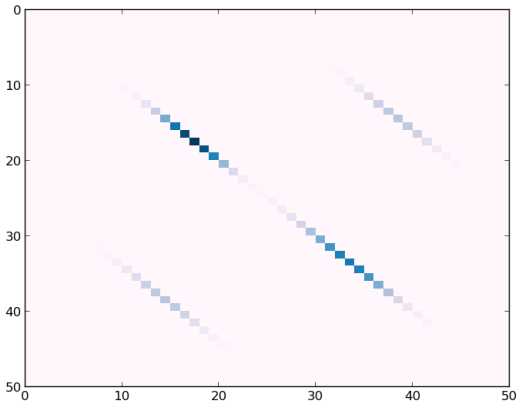
$$\begin{aligned}
\dot\rho(u,v) = \langle u|\dot\rho|v\rangle &= -\frac{i\omega'}{\hbar}\langle u|(a^\dagger a\rho_S - \rho_S a^\dagger a)|v\rangle + \gamma_1\langle u|(a\rho_S a^\dagger - \frac{1}{2}a^\dagger a\rho_S - \frac{1}{2}\rho_S a^\dagger a)|v\rangle \\
&+ \gamma_2\langle u|(a^\dagger\rho_S a - \frac{1}{2}aa^\dagger\rho_S - \frac{1}{2}\rho_S aa^\dagger)|v\rangle \\
&= -\frac{i\omega'}{\hbar}(u^\star(\frac{1}{2}u + \frac{d}{du^\star})\langle u|\rho_S|v\rangle - v\langle u|\rho_S(\frac{1}{2}v^\star + \frac{d}{dv})|v\rangle) \\
&+ \gamma_1((\frac{1}{2}u + \frac{d}{du^\star})\langle u|\rho_S(\frac{1}{2}v^\star + \frac{d}{dv})|v\rangle - \frac{1}{2}u^\star(\frac{1}{2}u + \frac{d}{du^\star})\langle u|\rho_S|v\rangle - \frac{1}{2}\langle u|\rho_S v(\frac{1}{2}v^\star + \frac{d}{dv})|v\rangle) \\
&+ \gamma_2(u^\star v\langle u|\rho_S|v\rangle - \langle u|\rho_S|v\rangle - \frac{1}{2}u^\star(\frac{1}{2}u + \frac{d}{du^\star})\langle u|\rho_S|v\rangle - \frac{1}{2}\langle u|\rho_S v(\frac{1}{2}v^\star + \frac{d}{dv})|v\rangle)
\end{aligned}$$



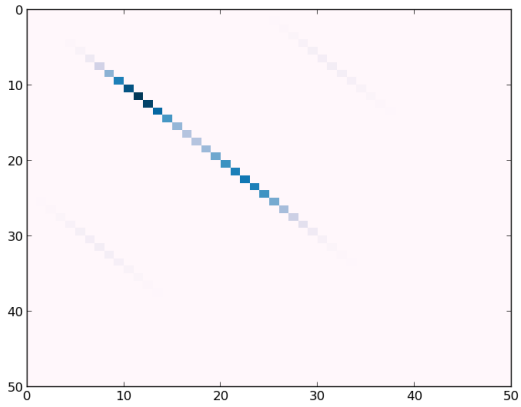
(a) $\gamma t = 0$



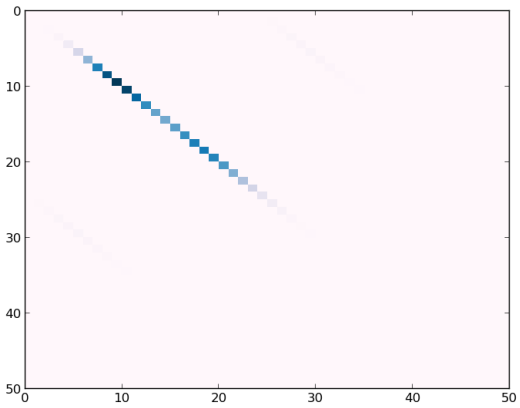
(b) $\gamma t = 0.05$



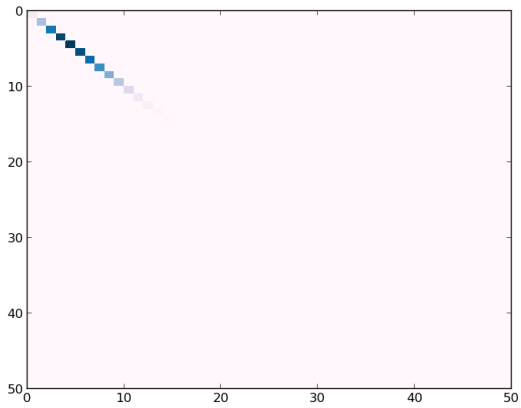
(c) $\gamma t = 0.2$



(d) $\gamma t = 0.4$



(e) $\gamma t = 0.5$



(f) $\gamma t = 1.0$

Figure 7.2: Plot of n-basis state matrix for different times t in a typical time development of a damped harmonic oscillator. The colors represents the magnitude of the matrix elements. Note how the non diagonal matrix elements are damped out with time relative to the diagonal ones, and how this happens faster for elements that are farther from the diagonal. By $\gamma t = 0.5$ non diagonal elements are no longer visible. Note also the behavior of the diagonal elements, which represents the probability of finding the oscillator in a particular n-state.

$$= -(\frac{\gamma_1+\gamma_2}{2}+i\omega)u^\star(\frac{1}{2}u+\frac{\partial}{\partial u^\star})\rho-(\frac{\gamma_1+\gamma_2}{2}-i\omega)v(\frac{1}{2}v^\star+\frac{\partial}{\partial v})\rho$$
$$+\gamma_1(\frac{1}{2}u+\frac{\partial}{\partial u^\star})(\frac{1}{2}v^\star+\frac{\partial}{\partial v})\rho+\gamma_2(u^\star v-1)\rho \tag{7.47}$$

We are as before interested in the operators $\mathcal{G}_t\ |z\rangle\langle w|$, which we will find by solving 7.21 with the initial value $|z\rangle\langle w|$. The initial value of $\rho(u,v)$ will then be $\rho(u,v)=\exp(-\frac{1}{2}(d(u,z)+d(w,v)))$. We will make an ansatz to the solution which is somewhat similar to this:

$$\rho(t,u,v)=A(t)\exp\left(-\frac{1}{2}B(t)(d(u,z(t))+d(w(t),v))+C(t)d(u,v)\right), \tag{7.48}$$

where $A(0)=B(0)=1$, $C(0)=0$, $z(0)=z$ and $w(0)=w$.

Inserting this ansatz into equation 7.47, then after an extensive amount of algebra we end up with the following eight equations which must be satisfied for the ansatz to be a solution.

$$\frac{\dot{A}}{A}+\frac{1}{2}\dot{B}(|z|^2+|w|^2)-\frac{1}{2}B(z^\star\dot{z}+w^\star\dot{w}+\dot{z}^\star z+\dot{w}^\star w)=-2\gamma_1C+\gamma_1B^2w^\star z-\gamma_2 \tag{7.49}$$

$$B-B^2+2BC=0 \tag{7.50}$$

$$\dot{B}z+B\dot{z}=-(\frac{\gamma_1+\gamma_2}{2}+i\omega)Bz-2\gamma_1BCz \tag{7.51}$$

$$\dot{B}w^\star+B\dot{w}^\star=-(\frac{\gamma_1+\gamma_2}{2}-i\omega)Bw^\star-2\gamma_1BCw^\star \tag{7.52}$$

$$1-2B+4C+B^2-4BC+4C^2=0 \tag{7.53}$$

$$-2\dot{C}=2(\gamma_1+\gamma_2)C+4\gamma_1C^2+\gamma_2 \tag{7.54}$$

$$-\frac{1}{2}\dot{B}+\dot{C}=-(\frac{\gamma_1+\gamma_2}{2}-i\omega)(\frac{1}{2}-\frac{1}{2}B+C)+\gamma_1(-C+BC-2C^2) \tag{7.55}$$

$$-\frac{1}{2}\dot{B}+\dot{C}=-(\frac{\gamma_1+\gamma_2}{2}+i\omega)(\frac{1}{2}-\frac{1}{2}B+C)+\gamma_1(-C+BC-2C^2) \tag{7.56}$$

We quickly see that the only interesting solution to 7.50 is $B=1+2C$, which also makes the equations 7.53, 7.55 and 7.56 immediately satisfied. Note that with this the number of remaining equations becomes equal to the number of remaining unknowns, which is something that should increase our faith in the ansatz.

Let us then turn to equation 7.54. This equation is expressed purely in terms of the unknown C, but let us reexpress it in terms of B. This gives us

$$\dot{B}=-2(\gamma_1+\gamma_2)\frac{B-1}{2}+4\gamma_1\frac{(B-1)^2}{4}-\gamma_2$$
$$=-(\gamma_1+\gamma_2)B+\gamma_1+\gamma_2-\gamma_1(B^2-2B+1)-\gamma_2$$
$$=(\gamma_1-\gamma_2)B-\gamma_1B^2. \tag{7.57}$$

Keeping in mind that $\gamma_1-\gamma_2=\gamma$ (see the definitions below 7.21)and that $B(0)=1$ we solve this separable equation as follows:

$$\int_0^t dt=t=\int_1^B\frac{dB}{(\gamma-\gamma_1B)B}=\frac{1}{\gamma}\int_1^B\left(\frac{1}{B}-\frac{\gamma_1}{\gamma_1B-\gamma}\right)dB$$
$$=\frac{1}{\gamma}(\ln B-\ln(\gamma_1B-\gamma)+\ln\gamma_2)=\frac{1}{\gamma}\ln\frac{B}{\frac{\gamma_1}{\gamma_2}B-\frac{\gamma}{\gamma_2}}. \tag{7.58}$$

From this it follows easily that $e^{\gamma t} = \frac{B}{\frac{\gamma_1}{\gamma_2}B - \frac{\gamma}{\gamma_2}}$, and then finally that

$$B = \frac{\frac{\gamma}{\gamma_2}e^{\gamma t}}{1 + \frac{\gamma_1}{\gamma_2}e^{\gamma t}} = \frac{\gamma}{\gamma_1 - \gamma_2 e^{-\gamma t}} = \frac{1}{1 + n(1 - e^{-\gamma t})} = \frac{1}{1+\chi}, \tag{7.59}$$

where we have made the definition $\chi = n(1 - e^{-\gamma t})$. We can now also find an explicit expression for C:

$$C = \frac{B-1}{2} = \frac{1}{2}\left(\frac{1}{1+\chi} - 1\right) = -\frac{1}{2}\left(\frac{\chi}{1+\chi}\right) \tag{7.60}$$

Next, we turn to equations 7.51 and 7.52. If we take the conjugate of 7.52, and then exchange w for z, we get 7.51. This means we really only need to solve one of these equations, so let us pick 7.51. Inserting $C = \frac{B-1}{2}$ as well as $\dot{B} = (\gamma_1 - \gamma_2)B - \gamma_1 B^2$ from 7.57, and then solving for $\dot{z}$ turns this equation into

$$\dot{z} = -\frac{1}{2}(\gamma_1 + \gamma_2 + 2i\omega)z + \gamma_1 z + (\gamma_2 - \gamma_1)z = -\frac{1}{2}(\gamma_1 - \gamma_2 + 2i\omega)z = -(\frac{\gamma}{2} + i\omega)z. \tag{7.61}$$

Given that $z(0) = z$, we find that the solution must be $z(t) = ze^{-(\gamma/2 + i\omega)t}$. From the argument above concerning the similarity between 7.51 and 7.52, we conclude also that $w(t) = we^{-(\gamma/2+i\omega)t}$. Note that the behavior of $z(t)$ and $w(t)$ is completely identical to what we found from solving 7.29 and 7.30 in the vacuum case.

Finally we turn to the first equation, 7.49. Inserting the obtained results $2C = B - 1$, $\dot{z} = -(\frac{\gamma}{2} + i\omega)z$, $\dot{w} = -(\frac{\gamma}{2} + i\omega)w$ as well as $B^2 = \frac{\gamma B - \dot{B}}{\gamma_1}$ from 7.57, we end up with the equation

$$\begin{aligned}
\frac{\dot{A}}{A} &= \frac{1}{2}\dot{B}(|z|^2 + |w|^2) - \frac{1}{2}B(\frac{\gamma}{2} + i\omega + \frac{\gamma}{2} - i\omega)(|z|^2 + |w|^2) - \gamma_1(B-1) + \gamma_1 w^\star z\frac{\gamma B - \dot{B}}{\gamma_1} - \gamma_2 \\
&= \frac{1}{2}(\dot{B} - \gamma B)(|z|^2 - 2w^\star z + |w|^2) - \gamma_1 B + \gamma = \frac{1}{2}(\dot{B} - \gamma B)d(w,z) + \frac{\gamma B - \gamma_1 B^2}{B} \\
&= \frac{\dot{B}}{B} + \frac{1}{2}(\dot{B} - \gamma B)d(w,z).
\end{aligned} \tag{7.62}$$

We then integrate this equation from $t = 0$ to t to get

$$\begin{aligned}
\ln A &= \ln B + \frac{1}{2}\int_0^t (\dot{B} - \gamma B)d(w(t), z(t))dt = \ln B + \frac{1}{2}d(w,z)\int_0^t (\dot{B} - \gamma B)e^{-\gamma t}dt \\
&= \ln B + \frac{1}{2}d(w,z)(Be^{-\gamma t} - 1),
\end{aligned} \tag{7.63}$$

so that

$$A = B\exp\left(\frac{1}{2}(Be^{-\gamma t} - 1)d(w,z)\right) = \frac{1}{1+\chi}\exp\left(\frac{1}{2}(\frac{e^{-\gamma t}}{1+\chi} - 1)d(w,z)\right). \tag{7.64}$$

Having now found expressions for all our ansatz parameters, we can finally set up the full solution. It is

$$\rho(t,u,v) = \frac{1}{1+\chi}\exp\left(-\frac{1}{2}\frac{1}{1+\chi}(d(u,zr) + d(wr,v) + \chi d(u,v)) + \frac{1}{2}(\frac{|r|^2}{1+\chi} - 1)d(w,z)\right), \tag{7.65}$$

$$\text{with } \chi = n(1 - e^{-\gamma t}), \tag{7.66}$$

$$\text{and } \; r = e^{-(\frac{\gamma}{2} + i\omega)t}. \tag{7.67}$$

In our analysis of this solution, let us begin by setting $w = z$, so that it actually corresponds to a valid state by it self. What we then get is

$$\rho(t,u,v) = \frac{1}{1+\chi}\exp\left(-\frac{1}{2}\frac{1}{1+\chi}(d(u,zr)+d(zr,v)+\chi d(u,v))\right). \tag{7.68}$$

To interpret this expression it might help to calculate $\langle u|\,\rho\,|v\rangle$ for a thermal state $\rho = (1-e^{-\beta\hbar\omega})e^{-\beta\hbar\omega a^\dagger a}$. Let us do this:

$$\begin{aligned}
\langle u|\,\rho\,|v\rangle &= (1-e^{-\beta\hbar\omega})\sum_n e^{-\beta\hbar\omega n}\langle u|n\rangle\langle n|v\rangle \\
&= (1-e^{-\beta\hbar\omega})\sum_n e^{-\beta\hbar\omega n}\frac{1}{n!}(u^\star v)^n e^{-\frac{1}{2}(|u|^2+|v|^2)} \\
&= (1-e^{-\beta\hbar\omega})e^{-\frac{1}{2}(|u|^2+|v|^2)}\exp(e^{-\beta\hbar\omega}u^\star v) \\
&= (1-e^{-\beta\hbar\omega})\exp\left(-\frac{1}{2}((1-e^{-\beta\hbar\omega})(|u|^2+|v|^2)+e^{-\beta\hbar\omega}d(u,v))\right) \\
&= (1-e^{-\beta\hbar\omega})\exp\left(-\frac{1}{2}((1-e^{-\beta\hbar\omega})(d(u,0)+d(0,v)+\frac{d(u,v)}{e^{\beta\hbar\omega}-1}))\right) \\
&= \frac{1}{1+n}\exp\left(-\frac{1}{2}\frac{1}{1+n}(d(u,0)+d(0,v)+nd(u,v))\right),
\end{aligned} \tag{7.69}$$

where as before $n = \langle n\rangle = 1/(e^{\beta\hbar\omega}-1)$. As we see, this expression is very similar to 7.68. The only differnece is that we must replace n with χ and shift the distribution by zr in complex plane. We conclude from this that 7.68 in fact represents nothing but a thermal state with $\langle n\rangle = \chi$ which is translated out by a coherent state index zr, so as to be centered around this value instead of the energy minimum at $z = 0$. Note also that χ approaches n, the number expectation value corresponding to the environmental temperature, as $t \to \infty$. This means that in this limit S will be in a thermal state with temperature equal to that of the environment, which is physically reasonable.

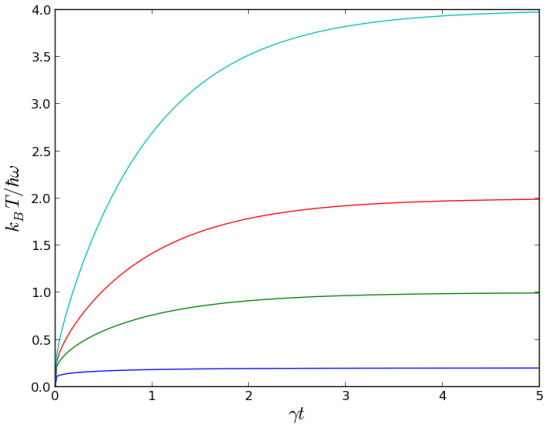
With this we can attempt to describe in words what happens to an oscillator in a coherent state when coupled to a thermal heat bath: The state will spiral inwards toward the origin of the complex plane, following precisely the same path as in the vacuum environment case. This damping of the oscillator will also happen just as fast as in the vacuum case. The only new effect introduced by finite temperature, is that the oscillator will be gradually heated in parallel with the damping. Starting out at zero, the temperature will grow to approach that of the environment.

It might be interesting to see precisely how this temperature changes with time. That is, to express the effective temperature as a function of time. Since we already know the dependence of χ, which is a sort of effective n, on time, this will not be difficult. Setting $\langle n\rangle = \chi = 1/(e^{\beta\hbar\omega}-1)$, we solve for β to get

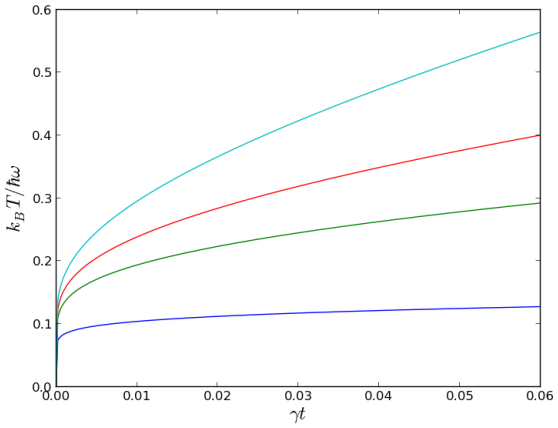
$$\begin{aligned}
\beta\hbar\omega &= \ln\left(1+\frac{1}{\chi}\right) = \ln\left(1+\frac{1}{n(1-e^{-\gamma t})}\right) \\
&= \ln\left(1+\frac{e^{\beta_E\hbar\omega}-1}{1-e^{-\gamma t}}\right) = \ln\left(\frac{e^{\beta_E\hbar\omega+\gamma t}-1}{e^{\gamma t}-1}\right),
\end{aligned} \tag{7.70}$$

$$T = \frac{1}{k_B\beta} = \frac{\hbar\omega}{k_B}\,\frac{1}{\ln\left((e^{\beta_E\hbar\omega+\gamma t}-1)/(e^{\gamma t}-1)\right)}, \tag{7.71}$$

where $1/k_B\beta_E = T_E$ now denotes the temperature of the environment. In ranges where $\frac{\hbar\omega}{k_B T_E} \ll 1-e^{-\gamma t}$ this result may be expanded as $T = (1-e^{-\gamma t})T_E$, which is the classical limit and follows newtons law of heating. The behavior when this condition is not met is shown in figure 7.3



(a) Temperature growth, long time behavior.



(b) Temperature growth, short time behavior.

Figure 7.3: Temperature as a function of time for harmonic oscillator coupled to heat bath at different environmental temperatures. These temperatures are $\frac{k_B T}{\hbar\omega} = 0.2$, 1.0, 2.0 and 4.0. The oscillators temperature approaches that of the environment for large times, and mostly it seems to follow the expected classical curve $T = (1 - e^{-\gamma t})T_E$. For very small times however, it deviates from this by an almost instantaneous rise in temperature. This is a non classical quantum result, which is due to the exponentially small heat capacity of a quantum harmonic oscillator at low temperatures.

Next, we again turn to examining decoherence, so that we can see whether finite temperature makes any changes to this. Obviously, the fact that we always end up in a thermal state means that no state remains pure, so in this sense we always have decoherence. This is of course something new relative to the vacuum situation, where a coherent state would remain pure. There is however another side to decoherence which we have looked at in particular in the previous subsections: The tendency of a superposition of states from a particular basis to approach a classical mix of states from this basis. This is something which would be interesting to look at also in the case of finite temperature, and in particular we would like to see if this happens in the coherent state basis. Obviously this will happen in the end, since all states will limit towards the equilibrium state. So what we are actually interested in is whether it happens considerably faster than the approach to equilibrium.

We found above that a coherent state after time t will be in a translated thermal state. Such a thermal state can indeed be expressed as a classical mix of coherent states. The question is however whether a pure state which is initially not a coherent state will limit towards such a mix (over fast timescales). Let us therefore once again assume that the oscillator begins in a superposition proportional to $|z\rangle + |w\rangle$. As before the state operator will be proportional to $|z\rangle\langle z| + |w\rangle\langle z| + |z\rangle\langle w| + |w\rangle\langle w|$, which with time will develop into $\mathcal{G}_t(|z\rangle\langle z|) + \mathcal{G}_t(|z\rangle\langle w|) + \mathcal{G}_t(|w\rangle\langle z|) + \mathcal{G}_t(|w\rangle\langle w|)$.

The difference between this state and and what we would get if we instead started out with a classical mix of the two states $|z\rangle$ and $|w\rangle$ is in the term $\mathcal{G}_t(|z\rangle\langle w|)$ and its Hermitian conjugate. Since we know that a classical mix of coherent states will remain a classical mix of coherent states, these terms are all that separates $\rho(t)$ from a such a classical mix. What we are essentially interested in then, is some quantity which indicates the magnitude or 'strength' of the term $\mathcal{G}_t(|z\rangle\langle w|)$. One quantity which would do this job, is the maximal value of the function $f(u,v) = |\langle u|\mathcal{G}_t(|z\rangle\langle w|)|v\rangle|$. This quantity, which we shall denote $c(t)$ is the one we will use. This is because it can be calculated easily from 7.65, and because it is a direct generalization of the quantity $|f(t)|$ used in the vacuum case analysis. To see this we calculate $\langle u|\mathcal{G}_t(|z\rangle\langle w|)|v\rangle = f(t)\langle u|z\rangle\langle w|v\rangle$, of which the maximal absolute value is indeed $|f(t)|$.

In the finite temperature case we find from 7.65 the absolute value of $\langle u|\mathcal{G}_t(|z\rangle\langle w|)|v\rangle$ to be

$$f(u,v) = \frac{1}{1+\chi}\exp\left(-\frac{1}{2}\frac{1}{1+\chi}(|u-zr|^2 + |wr-v|^2 + \chi|u-v|^2) + \frac{1}{2}(\frac{|r|^2}{1+\chi} - 1)|z-w|^2\right). \quad (7.72)$$

The maximal value is obviously determined by the terms containing u and v, that is $|u - zr|^2 + |wr - v|^2 + \chi|u - v|^2$. The maximal value of this can be found from differentiating, and setting the derivatives to zero. We should differentiate both with respect to u and v themselves and their conjugates, which would result in four equations. However, these equation will be pairwise conjugate, so really we only need differentiate with respect to for instance $u^\star$ and v. This results in the two equations

$$(1+\chi)u - rz - \chi v = 0, \tag{7.73}$$

$$(1+\chi)v - rw - \chi u = 0. \tag{7.74}$$

Being simple linear equations, these are easy to solve and their solutions are

$$u = \frac{wr + \chi(z+w)r}{1+2\chi}, \tag{7.75}$$

$$v = \frac{zr + \chi(z+w)r}{1+2\chi}. \tag{7.76}$$

From this we calculate

$$u - zr = \frac{wr + \chi(z+w)r - zr - 2\chi zr}{1+2\chi} = \frac{\chi r(z-w)}{1+2\chi}, \tag{7.77}$$

$$v - wr = \frac{zr + \chi(z+w)r - zr - 2\chi wr}{1+2\chi} = \frac{\chi r(w-z)}{1+2\chi}, \tag{7.78}$$

$$u - v = \frac{wr + \chi(z+w)r - zr - \chi(z+w)r}{1+2\chi} = \frac{r(z-w)}{1+2\chi}, \tag{7.79}$$

and inserting this in 7.72, we get

$$\begin{aligned} c(t) &= \exp\left(-\frac{1}{2}\frac{|r|^2}{1+\chi}\left(2\cdot\frac{\chi^2}{(1+2\chi)^2} + \chi\cdot\frac{1}{(1+2\chi)^2} - 1\right)|z-w|^2 - \frac{1}{2}|z-w|^2\right) \\ &= \exp\left(-\frac{1}{2}\frac{|r|^2}{1+\chi}\left(\frac{\chi}{1+2\chi} - 1\right)|z-w|^2 - \frac{1}{2}|z-w|^2\right) \\ &= \exp\left(-\frac{1}{2}\left(1 - \frac{|r|^2}{1+2\chi}\right)|z-w|^2\right) \end{aligned} \tag{7.80}$$

where the factor $1/(1+\chi)$ has been excluded in order to make the expression equal to 1 when $z = w$. We note that for $T = \chi = 0$, the expression does indeed reduce to $c(t) = e^{-\frac{1}{2}(1-|r|^2)|z-w|^2}$, which was what we found in the vacuum case.

In the limit of weak interactions in particular, we get from 7.66 and 7.67 that

$$c(t) = \exp\left(-\frac{1}{2}\left(1 - \frac{e^{-\gamma t}}{1+2n(1-e^{-\gamma t})}\right)|z-w|^2\right). \tag{7.81}$$

Examples of the development of $c(t)$ can be seen in figure 7.4. In addition to this, it is interesting to analyze the behavior of the function in the limits where $\gamma t \gg 1$ or $\gamma t \ll 1$. It is easily seen that when $\gamma t \gg 1$ $c(t) \to e^{-\frac{1}{2}|z-w|^2}$, the overlap of the states $|z\rangle$ and $|w\rangle$. Seemingly, finite temperature brings nothing new here relative to the vacuum case. In the $\gamma t \ll 1$ limit however, there is a difference. Or more precisely, in the limit where both $\gamma t \ll 1$ and $n\gamma t \ll 1$. If this is the case, 7.82 may be expanded in the following way:

$$c(t) \approx \exp\left(-\frac{1}{2}\left(1 - (1-\gamma t)(1-2n\gamma t)\right)|z-w|^2\right) \approx \exp\left(-\frac{1}{2}(1+2n)\gamma t|z-w|^2\right). \tag{7.82}$$

We note that for finite temperature, the instantaneous decay rate of the coherence is $-\frac{1}{2}(1+2n)\gamma|z-w|^2$, which is larger by a factor $1+2n = \frac{e^{\beta\hbar\omega}+1}{e^{\beta\hbar\omega}-1}$ than the vacuum result. In the high temperature limit this factor is $2k_BT/\hbar\omega$.

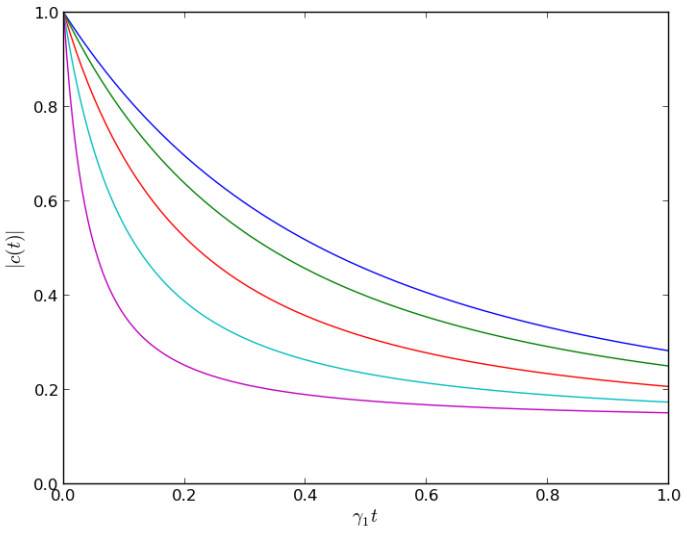


Figure 7.4: Plot of the $c(t)$ against $\gamma_1 t$. All graphs have $|z - w| = 2$, but the temperature is varied. The blue, green, red, cyan and purple curves are respectively calculated with $k_B T/\hbar\omega = 0$, 0.5, 1.0, 2.0 and 5.0. Note that that all curves seem to limit towards the same value, but that the initial decay rate increases with temperature.

7.4 Exact solution

Until now, all calculations of time development have been made using the Redfield/Lindblad equation, and so they are only valid in the weak interaction limit. In this subsection we will therefor solve the model defined by Hamiltonian 7.1 exactly. This will allow us to generalize our results, as well as to analyze how well the Redfield approximation actually performs in the weak interaction limit. We will find that in fact the formulas 7.33 and 7.65 generalize to the exact solution. The only thing new is that the parameters r and χ are no longer given by the same simple exponential expressions.

Physically this generalization is not very interesting, as we have already assumed weak interactions at the level of the Hamiltonian: There it was assumed that the interactions are weak compared to the oscillators energy scale $\hbar\omega$, which was what allowed us to employ the rotating wave approximation. The Redfield equation demands the interactions to be weak in comparison to the environmental energy range. Clearly then, the particular generalization to be made here would only be interesting in cases where the interactions are comparable to the environmental energy scale but not to that of the system S. Typically the environmental energy range is much larger than that of S, so that this is impossible.

Generalizing the results of this model to strong interactions is thus not interesting due to a desire to compare it with realistic physical systems, but rather because we can study the performance of the Redfield approximation and because we may get some hints of the general consequences of moving away from the weak interaction limit. Also, this model has an advantage in that the exact solution follows from a very simple diagonalization approach. In the literature one can find several treatments of more realistic strongly interacting oscillators, such as for instance the famous Cadeira Legett model[2][3].

7.4.1 Coherent state environment

Let us begin by assuming that the total system $T = S \otimes E$ is initially in the state $|\boldsymbol{z}\rangle = |z\rangle \otimes \prod_i |z_i\rangle$, where $|z\rangle$ is a coherent state of S, $|z_i\rangle$ is a coherent state of the environmental oscillator i and $\boldsymbol{z}$ is a vector with z as its zeroth component and z_i as its i'th component. The time development will remain in the same form $|\boldsymbol{z}(t)\rangle$, as can be shown by inserting this ansatz in the Schrodinger equation. The time

derivative is found from 7.26:

$$\frac{d}{dt}|\boldsymbol{z}\rangle = \sum_i \left(\prod_{j\neq i}|z_j\rangle\right)\otimes\frac{d}{dt}|z_i\rangle = \sum_i \left(\prod_{j\neq i}|z_j\rangle\right)\otimes(-\mathcal{R}ez_i^\star\dot{z}_i + \dot{z}_i a_i^\dagger)|z_i\rangle = (-\mathcal{R}e\boldsymbol{z}^\dagger\dot{\boldsymbol{z}} + \boldsymbol{a}^\dagger\dot{\boldsymbol{z}})|\boldsymbol{z}\rangle\,. \tag{7.83}$$

Inserting this and the Hamiltonian 7.3 in the Schrodinger equation, we get

$$\hbar i(-\mathcal{R}e\boldsymbol{z}^\dagger\dot{\boldsymbol{z}} + \boldsymbol{a}^\dagger\dot{\boldsymbol{z}})|\boldsymbol{z}\rangle = \boldsymbol{a}^\dagger W\boldsymbol{a}|\boldsymbol{z}\rangle = \boldsymbol{a}^\dagger W\boldsymbol{z}|\boldsymbol{z}\rangle\,, \tag{7.84}$$

where the matrix W is defined in 7.2. This equation will be satisfied if

$$\mathcal{R}e\boldsymbol{z}^\dagger\dot{\boldsymbol{z}} = 0, \text{ and} \tag{7.85}$$

$$\dot{\boldsymbol{z}} = -\frac{i}{\hbar}W\boldsymbol{z}. \tag{7.86}$$

The lower of these equations actually implies that $\boldsymbol{z}^\dagger\dot{\boldsymbol{z}} = -i\boldsymbol{z}^\dagger W\boldsymbol{z}/\hbar$, which is purely imaginary when W is a Hermitian matrix. Thus, the upper equation is in fact implied by the lower, and all we need to do is to find a solution to this. This is simply

$$\boldsymbol{z}(t) = e^{-iWt/\hbar}\boldsymbol{z} = R(t)\boldsymbol{z}, \tag{7.87}$$

where we have defined $R(t) = e^{-iWt/\hbar}$. Note that the procedure to calculate $R(t)\boldsymbol{z}$ would typically be to express $\boldsymbol{z}$ in terms of eigenvectors of W. Thus, what we are essentially doing in 7.87 is to decouple the oscillators by diagonalization.

The time development of the total system T can now be expressed as

$$U(t)|\boldsymbol{z}\rangle = |\boldsymbol{z}(t)\rangle = |R(t)\boldsymbol{z}\rangle = |z(t)\rangle\otimes|\boldsymbol{z}_E(t)\rangle\,, \tag{7.88}$$

where $|\boldsymbol{z}_E(t)\rangle$ is a coherent state of the environment alone. Direct expressions for $z(t)$ and $\boldsymbol{z}_E(t)$ can be found if we decompose the matrix $R(t)$ in the following way:

$$R = \begin{pmatrix} r & \boldsymbol{r}_{0E}^\dagger \\ \boldsymbol{r}_{E0} & R_E \end{pmatrix}, \tag{7.89}$$

which makes

$$\begin{pmatrix} z(t) \\ \boldsymbol{z}_E(t) \end{pmatrix} = \begin{pmatrix} r & \boldsymbol{r}_{0E}^\dagger \\ \boldsymbol{r}_{E0} & R_E \end{pmatrix}\begin{pmatrix} z \\ \boldsymbol{z}_E \end{pmatrix} = \begin{pmatrix} rz + \boldsymbol{r}_{0E}^\dagger\boldsymbol{z}_E \\ z\boldsymbol{r}_{E0} + R_E\boldsymbol{z}_E \end{pmatrix}. \tag{7.90}$$

Knowing the development of T, we can now turn to the development of the reduced system S. Taking $\mathcal{G}_t$ to be defined by 3.2 and applying 7.88 we find that in the case that E starts out in some coherent state $|\boldsymbol{z}_E\rangle$ we will have

$$\begin{aligned}\mathcal{G}_t\,|z\rangle\langle w| &= \mathrm{Tr}_E U(t)|z\rangle\langle w|U(t)^\dagger = \mathrm{Tr}_E|z(t)\rangle\langle w(t)|\otimes|\boldsymbol{z}_E(t)\rangle\langle\boldsymbol{w}_E(t)| \\ &= |z(t)\rangle\langle w(t)|\cdot\langle\boldsymbol{w}_E(t)|\boldsymbol{z}_E(t)\rangle.\end{aligned} \tag{7.91}$$

The inner product $\langle\boldsymbol{w}_E(t)|\boldsymbol{z}_E(t)\rangle$ may be calculated as follows

$$\begin{aligned}\langle\boldsymbol{w}_E(t)|\boldsymbol{z}_E(t)\rangle &= \prod_i\langle w_i(t)|z(t)\rangle = \prod_i\exp\left(-\frac{1}{2}(|w_i(t)|^2 - 2w_i^\star(t)z_i(t) + |z_i(t)|^2)\right) \\ &= \exp\left(-\frac{1}{2}(|\boldsymbol{w}_E(t)|^2 - 2\boldsymbol{w}_E^\dagger(t)\boldsymbol{z}_E(t) + |\boldsymbol{w}_E(t)|^2)\right)\end{aligned} \tag{7.92}$$

This can be re-expressed by noting that R is a unitary matrix, so that

$$w^\star(t)z(t) + \boldsymbol{w}_E^\dagger(t)\boldsymbol{z}_E(t) = \boldsymbol{w}^\dagger(t)\boldsymbol{z}(t) = \boldsymbol{w}^\dagger R^\dagger(t)R(t)\boldsymbol{z} = \boldsymbol{w}^\dagger\boldsymbol{z} = w^\star z + |\boldsymbol{z}_E|^2. \tag{7.93}$$

This means that

$$\boldsymbol{w}_E^\dagger(t)\boldsymbol{z}_E(t) = |\boldsymbol{z}_E|^2 + w^\star z - w^\star(t)z(t), \tag{7.94}$$

so that in fact

$$\begin{aligned}\langle \boldsymbol{w}_E(t)|\boldsymbol{z}_E(t)\rangle &= \exp\left(-\frac{1}{2}(|\boldsymbol{w}_E(t)|^2 - 2\boldsymbol{w}_E^\dagger(t)\boldsymbol{z}_E(t) + |\boldsymbol{w}_E(t)|^2)\right)\\ &= \exp\left(-\frac{1}{2}(|\boldsymbol{z}_E|^2 + |w|^2 - |w(t)|^2 - 2|\boldsymbol{z}_E|^2 - 2w^\star z + 2w^\star(t)z(t) + |\boldsymbol{z}_E|^2 + |z|^2 - |z(t)|^2)\right)\\ &= \exp\left(-\frac{1}{2}\left(d(w,z) - d(w(t),z(t))\right)\right)\end{aligned} \tag{7.95}$$

With this we can finally write down

$$\mathcal{G}_t\ |z\rangle\langle w| = |z(t)\rangle\langle w(t)| \cdot \exp\left(-\frac{1}{2}\left(d(w,z) - d(w(t),z(t))\right)\right). \tag{7.96}$$

In particular, if the environment is initially in the vacuum state so that $\boldsymbol{z}_E = \boldsymbol{0}$, 7.90 tels us that

$$\mathcal{G}_t\ |z\rangle\langle w| = |zr\rangle\langle wr| \cdot e^{-\frac{1}{2}(1-|r|^2)d(w,z)}. \tag{7.97}$$

This expression is seen to be completely identical to 7.33. The only difference is that $r(t)$ is no longer given by the simple Markovian formula $r = e^{-\frac{\gamma}{2}t - i\omega t}$.

So how will the quantity $r(t)$ develop in the exact solution? Well, in this case $r(t)$ is given as the 00 component of the matrix $R(t) = e^{-iWt/\hbar}$. By comparing the Hamiltonian of this model with the two-level model of the previous section, one will find that the matrix W has precisely the same form as the matrix representation of the Hamiltonian 6.1 of the previous chapter. If the corresponding parameters are chosen to be equal, these two matrices will even be identical. This also means that the matrix $R(t)$ will be identical to the matrix representation of the time development operator $U(t)$ of this model, and in particular the 00 components of these matrices will be equal.

With other words $r(t)$ will be identical to the quantity which in the previous section was denoted $c(t)$, and which there was the primary object of investigation. Because we have already devoted an entire section to the analysis of this quantity, we will not say much about it here. The only thing we will note is the important point that in the markovian limit we indeed found $c(t)$ and thus also $r(t)$ to have the simple exponential form $e^{-\frac{\gamma}{2}t - i\omega t}$. We also note that since 7.97 is identical to 7.33, all formulas and conclusions derived from this continue to apply in the exact solution. Except of course for the ones which explicitly depends on the exponential form of $r(t)$.

7.4.2 Thermal environment

Seeing then that there is not much more to say about the vacuum environment case, we turn to the finite temperature situation. We assume then that the environment E is initially in the thermal state $\frac{1}{Z}e^{-\beta H_E}$, and once again we calculate $\mathcal{G}_t(|z\rangle\langle w|)$. The first step is to express the thermal state of the environment in terms of coherent states. A thermal state of a single oscillator may be expressed as

$$\rho = (1 - e^{-\beta\hbar\omega})e^{-\beta\hbar\omega N} = \frac{1}{\pi n}\int e^{-|z|^2/n}\,|z\rangle\langle z|\,d^2z, \tag{7.98}$$

where again $n = 1/(e^{\beta\hbar\omega} - 1)$. The first equality is taken from 2.39. By again employing the formula 2.46, the second can be shown as follows:

$$\begin{aligned}
&\langle m| \frac{1}{\pi n} \int e^{-|z|^2/n} |z\rangle \langle z| d^2z |l\rangle = \frac{1}{\pi n} \int e^{-|z|^2/n} \langle m|z\rangle\langle w|l\rangle d^2z \\
&= \frac{1}{\pi n\sqrt{m!l!}} \int z^m z^{\star l} e^{-|z|^2/n - |z|^2} d^2z = \frac{1}{\pi n\sqrt{ml}} \int r^{2l} e^{-(n+1)r^2/n} \int z^{m-l} d\theta r dr \\
&= \frac{1}{\pi n m!} 2\pi \frac{m!}{2} \left(\frac{n}{n+1}\right)^{m+1} \delta_{ml} = \frac{1}{n+1} \left(\frac{n}{n+1}\right)^{m} \delta_{ml} = (1 - e^{-\beta\hbar\omega}) e^{-\beta\hbar\omega m} \delta_{ml}, \qquad (7.99)
\end{aligned}$$

just as it would be for $(1 - e^{-\beta\hbar\omega})e^{-\beta\hbar\omega N}$. Thus, it is clear that the initial state of E is

$$\rho_E(0) = \prod_i \frac{1}{\pi n_i} \int e^{-|z|^2/n_i} |z_i\rangle \langle z_i| d^2z_i = \frac{1}{\pi^m \det(N)} \int e^{-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z}} |\boldsymbol{z}\rangle \langle \boldsymbol{z}| d^{2m}\boldsymbol{z}, \qquad (7.100)$$

where m is now the number of oscillators in the environment, and we have defined a diagonal matrix N having the expectation values n_i of the environmental oscillators on the diagonal.

With this we may use our previous result 7.96 to calculate

$$\begin{aligned}
\mathcal{G}_t(|z\rangle \langle w|) =& \mathrm{Tr}_E U(t) \left(|z\rangle \langle w| \otimes \frac{1}{\pi^m \det(N)} \int e^{-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z}} |\boldsymbol{z}\rangle \langle \boldsymbol{z}| d^{2m}\boldsymbol{z} \right) U(t)^\dagger \\
&= \frac{1}{\pi^m \det(N)} \int e^{-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z}} \mathrm{Tr}_E U(t) \left(|z\rangle \langle w| \otimes |\boldsymbol{z}\rangle \langle \boldsymbol{z}| \right) U(t)^\dagger d^{2m}\boldsymbol{z} \\
&= \frac{1}{\pi^m \det(N)} \int |z(t)\rangle\langle w(t)| \cdot \exp\left(-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z} - \frac{1}{2} \left(d(w,z) - d(w(t), z(t)) \right) \right) d^{2m}\boldsymbol{z}. \qquad (7.101)
\end{aligned}$$

In order to compare with the Markovian calculation, we will again calculate the complex numerical quantity $\langle u| \mathcal{G}_t(|z\rangle \langle w|) |v\rangle$. I must warn that this is a rather long calculation. By using the formula 2.47 together with 7.101 we get

$$\begin{aligned}
\langle u| \mathcal{G}_t(|z\rangle \langle w|) |v\rangle =& \frac{1}{\pi^m \det(N)} \int \langle u|z(t)\rangle\langle w(t)|v\rangle \cdot \exp\left(-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z} - \frac{1}{2} \left(d(w,z) - d(w(t), z(t)) \right) \right) d^{2m}\boldsymbol{z} \\
=& \frac{1}{\pi^m \det(N)} \int \exp\Big(-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z} - \frac{1}{2} (d(u, z(t)) + d(w(t), v) + d(w,z) \\
& - d(w(t), z(t))) \Big) d^{2m}\boldsymbol{z} \\
=& \frac{1}{\pi^m \det(N)} \int \exp\Big(-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z} - \frac{1}{2} (|u|^2 - 2u^\star z(t) - 2w^\star(t) v + |v|^2 \\
& + |z|^2 - 2w^\star z + |w|^2 + 2w^\star(t) z(t)) \Big) d^{2m}\boldsymbol{z} \\
=& \frac{1}{\pi^m \det(N)} \int \exp\Big(-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z} - \frac{1}{2} (|u|^2 + |v|^2 + |z|^2 + |w| - 2u^\star r z - 2u^\star \boldsymbol{r}^\dagger \boldsymbol{z} \\
& - 2r^\star w^\star v - 2\boldsymbol{z}^\dagger \boldsymbol{r} v - 2w^\star z + 2(w^\star r^\star + \boldsymbol{z}^\dagger \boldsymbol{r})(r z + \boldsymbol{z}^\dagger \boldsymbol{r})) \Big) d^{2m}\boldsymbol{z} \\
=& \frac{1}{\pi^m \det(N)} \int \exp\Big(-\boldsymbol{z}^\dagger N^{-1} \boldsymbol{z} - \frac{1}{2} (|u|^2 + |v|^2 + |z|^2 + |w|) + u^\star r z + u^\star \boldsymbol{r}^\dagger \boldsymbol{z}
\end{aligned}$$

$$+ r^\star w^\star v + \boldsymbol{z}^\dagger \boldsymbol{r} v + w^\star z - w^\star z|r|^2 - w^\star r^\star \boldsymbol{r}^\dagger \boldsymbol{z} - \boldsymbol{z}^\dagger \boldsymbol{r} r z - |\boldsymbol{z}^\dagger \boldsymbol{r}|^2 \Big) d^{2m}\boldsymbol{z}$$

$$= \frac{1}{\pi^m \det(N)} \exp\left(-\frac{1}{2}(|u|^2 + |v|^2 + |z|^2 + |w|) + u^\star r z + r^\star w^\star v + w^\star z(1 - |r|^2)\right)$$

$$\cdot \int \exp\Big(-\boldsymbol{z}^\dagger (N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)\boldsymbol{z} + (u^\star - w^\star r^\star)\boldsymbol{r}^\dagger \boldsymbol{z} + \boldsymbol{z}^\dagger \boldsymbol{r}(v - rz)\Big) d^{2m}\boldsymbol{z} \tag{7.102}$$

In order to explicitly compute this integral, we first note that the matrix M, which we define as $M = N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger$ is Hermitian and positively definite. This means we can construct a unitary matrix S which diagonalizes this matrix as $D = S^\dagger M S$, and further that all D_i are positive. We perform the integral by doing the coordinate transformation $\boldsymbol{z} \to S\boldsymbol{z}$. Note that since S is a unitary matrix, this transformation will not change the volume element $d^{2m}\boldsymbol{z}$.

$$\frac{1}{\pi^m} \int \exp\Big(-\boldsymbol{z}^\dagger (N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)\boldsymbol{z} + (u^\star - w^\star r^\star)\boldsymbol{r}^\dagger \boldsymbol{z} + \boldsymbol{z}^\dagger \boldsymbol{r}(v - rz)\Big) d^{2m}\boldsymbol{z}$$

$$= \frac{1}{\pi^m} \int \exp\Big(-\boldsymbol{z}^\dagger D\boldsymbol{z} + (u^\star - w^\star r^\star)\boldsymbol{r}^\dagger S\boldsymbol{z} + \boldsymbol{z}^\dagger S^\dagger \boldsymbol{r}(v - rz)\Big) d^{2m}\boldsymbol{z}$$

$$= \prod_i \frac{1}{\pi} \int \exp\Big(-D_i|z|^2 + (u^\star - w^\star r^\star)(\boldsymbol{r}^\dagger S)_i z + z^\star (S^\dagger \boldsymbol{r})_i (v - rz)\Big) d^2 z \tag{7.103}$$

The individual factors of this expression are all on the form $\frac{1}{\pi}\int e^{-a|z|^2 + bz + cz^\star} d^2 z$. These may be calculated using the same technique as 7.38:

$$\frac{1}{\pi} \int e^{-a|z|^2 + bz + cz^\star} d^2 z = \frac{1}{\pi} \int e^{-a|z - c/a|^2 + (b - c^\star)z + |c|^2/a} d^2 z = \frac{1}{\pi} \int e^{-a|z|^2 + (b-c^\star)(z + c/a) + |c|^2/a} d^2 z$$

$$= \frac{e^{bc/a}}{\pi} \int e^{-a|z|^2 + (b - c^\star)z} d^2 z = \frac{e^{bc/a}}{\pi} \int \oint e^{-ar^2 + (b-c^\star)z} r \frac{dz}{iz} dr$$

$$= e^{bc/a} \cdot \int_0^\infty r e^{-ar^2} \cdot 2\pi e^{(b - c^\star)0} = \frac{1}{a} e^{bc/a}, \tag{7.104}$$

so that

$$\frac{1}{\pi^m} \int \exp\Big(-\boldsymbol{z}^\dagger (N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)\boldsymbol{z} + (u^\star - w^\star r^\star)\boldsymbol{r}^\dagger \boldsymbol{z} + \boldsymbol{z}^\dagger \boldsymbol{r}(v - rz)\Big) d^{2m}\boldsymbol{z} =$$

$$\prod_i \frac{1}{D_i} \exp\left(\frac{(u^\star - w^\star r^\star)(\boldsymbol{r}^\dagger S)_i (S^\dagger \boldsymbol{r})_i (v - rz)}{D_i}\right) =$$

$$\frac{1}{\det(D)} \exp\Big((u^\star - w^\star r^\star)(v - rz)\boldsymbol{r}^\dagger S D^{-1} S^\dagger \boldsymbol{r}\Big) =$$

$$\frac{1}{\det(M)} \exp\Big((u - wr)^\star (v - rz)\boldsymbol{r}^\dagger M^{-1} \boldsymbol{r}\Big). \tag{7.105}$$

Inserting this in 7.102, we now get

$$\langle u| \mathcal{G}_t(|z\rangle \langle w|) |v\rangle = \frac{1}{\det(N)\det(M)} \exp\Big(-\frac{1}{2}(|u|^2 + |v|^2 + |z|^2 + |w|) + u^\star r z + r^\star w^\star v$$

$$+ w^\star z(1 - |r|^2) + (u - wr)^\star (v - rz)\boldsymbol{r}^\dagger M^{-1} \boldsymbol{r}\Big). \tag{7.106}$$

With this, we are almost done. The only thing that remains is to explicitly calculate the quantities $\det(N)\det(M)$ and $\boldsymbol{r}^\dagger M^{-1}\boldsymbol{r}$. Let us begin with the determinant. We can rewrite this

$$\det(N)\det(M) = \det(N^{\frac{1}{2}})^2\det(M) = \det(N^{\frac{1}{2}}MN^{\frac{1}{2}}) \tag{7.107}$$

$$= \det(N^{\frac{1}{2}}(N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)N^{\frac{1}{2}}) = \det(I + N^{\frac{1}{2}}\boldsymbol{r}\boldsymbol{r}^\dagger N^{\frac{1}{2}}). \tag{7.108}$$

Next we note that the only non zero eigenvalue of the matrix $N^{\frac{1}{2}}\boldsymbol{r}\boldsymbol{r}^\dagger N^{\frac{1}{2}}$ is $\boldsymbol{r}^\dagger N\boldsymbol{r}$, which belongs to the eigenvector $N^{\frac{1}{2}}\boldsymbol{r}$. Accordingly, $I + N^{\frac{1}{2}}\boldsymbol{r}\boldsymbol{r}^\dagger N^{\frac{1}{2}}$ has an eigenvalue $1 + \boldsymbol{r}^\dagger N\boldsymbol{r}$ of multiplicity 1, while all other eigenvalues are 1. This means that $\det(N)\det(M) = 1 + \boldsymbol{r}^\dagger N\boldsymbol{r}$.

Next, we shall want to calculate $\boldsymbol{r}^\dagger M^{-1}\boldsymbol{r} = \boldsymbol{r}^\dagger(N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)^{-1}\boldsymbol{r}$. This is easily done by noting that

$$\frac{(N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)N\boldsymbol{r}}{1 + \boldsymbol{r}^\dagger N\boldsymbol{r}} = \frac{\boldsymbol{r} + \boldsymbol{r}^\dagger N\boldsymbol{r}\cdot\boldsymbol{r}}{1 + \boldsymbol{r}^\dagger N\boldsymbol{r}} = \boldsymbol{r}, \tag{7.109}$$

which means that in fact

$$\boldsymbol{r}^\dagger(N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)^{-1}\boldsymbol{r} = \frac{\boldsymbol{r}^\dagger(N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)^{-1}(N^{-1} + \boldsymbol{r}\boldsymbol{r}^\dagger)N\boldsymbol{r}}{1 + \boldsymbol{r}^\dagger N\boldsymbol{r}} = \frac{\boldsymbol{r}^\dagger N\boldsymbol{r}}{1 + \boldsymbol{r}^\dagger N\boldsymbol{r}}. \tag{7.110}$$

If we now define

$$\chi = \boldsymbol{r}^\dagger N\boldsymbol{r} = \sum_i n_i|r_i|^2, \tag{7.111}$$

we can finally rewrite 7.106 as

$$\begin{aligned}
\langle u|\,\mathcal{G}_t(|z\rangle\langle w|)\,|v\rangle =& \frac{1}{\det(N)\det(M)}\exp\Big(-\frac{1}{2}(|u|^2 + |v|^2 + |z|^2 + |w|^2) + u^\star rz + r^\star w^\star v + w^\star z(1 - |r|^2) \\
&+ (u - wr)^\star(v - rz)\boldsymbol{r}^\dagger M^{-1}\boldsymbol{r}\Big) \\
=& \frac{1}{1+\chi}\exp\Big(-\frac{1}{2}(|u|^2 + |v|^2 + |z|^2 + |w|^2) + u^\star rz + r^\star w^\star v + w^\star z(1 - |r|^2) \\
&+ \frac{\chi}{1+\chi}(u^\star v - u^\star rz - w^\star r^\star v + w^\star z|r|^2)\Big) \\
=& \frac{1}{1+\chi}\exp\Big(-\frac{1}{2}\frac{1}{1+\chi}\big((1+\chi)(|u|^2 + |v|^2 + |z|^2 + |w|^2 - 2w^\star z) - 2u^\star rz \\
&- 2r^\star w^\star v + 2|r|^2 w^\star z - 2\chi u^\star v\big)\Big) \\
=& \frac{1}{1+\chi}\exp\Big(-\frac{1}{2}\frac{1}{1+\chi}\big(|u|^2 - 2u^\star rz + |rz|^2 + |v|^2 - 2r^\star w^\star v + |rw|^2 \\
&- |rz|^2 + 2|r|^2 w^\star z - |rw|^2 + \chi(|u|^2 - 2u^\star v + |v|^2)\big) - \frac{1}{2}(|z|^2 - 2w^\star z + |w|^2)\Big) \\
=& \frac{1}{1+\chi}\exp\left(-\frac{1}{2}\frac{1}{1+\chi}(d(u, zr) + d(wr, v) + \chi d(u, v)) + \frac{1}{2}(\frac{|r|^2}{1+\chi} - 1)d(w, z)\right).
\end{aligned} \tag{7.112}$$

Once again, we see that this expression is completely identical to our findings in the Markovian approximation, that is 7.65. However, as before the involved parameters does not behave in the same simple manor. That is, r and χ are no longer given by the simple exponential formulas of 7.67 and 7.66.

$r(t)$ is still the 00 component of the R matrix, and our conclusion that the z expectation value follows the same path at finite temperature as in the zero temperature case still applies in the exact solution. The behavior of this parameter will therefore not be further discussed in this section either. The behavior of the parameter χ however we have as of yet not studied in the exact case, where it is given by 7.111. This parameter is still connected to the effective temperature of the oscillator by the formula $\chi = 1/(e^{\beta\hbar\omega} - 1)$, and its behavior thus tells us about the heat flow between the oscillator and its environment. The behavior of χ for a few illustrating environmental specifications are shown in figure 7.5, where it is compared with the Markovian formula $\chi = n(1 - e^{-\gamma t})$.

Even though χ will obviously not obey this formula, one could imagine it would follow a sort of minimal generalization of this, namely $\chi = n(1 - |r|^2)$. If this was the case, the mechanical damping and heating would not be independent. As long as one knows the temperature of the environment, one could easily calculate one from the other. In order to see whether this is the case or not, the simple generalization $\chi = n(1 - |r|^2)$ is also shown in the figure.

The first thing we may note from the figure, is that the Markovian formula does seem to fit very well in the weak interaction limit. Secondly we note that the naive generalization in all of the cases lies much closer to the Markovian formula itself, than to the actual development of χ. It is therefore completely useless. In fact, it seems we must conclude from figure 7.5 that the effects of stronger interactions are much larger on the thermal development represented by χ than they are on the mechanical decay. While the mechanical parameters does not significantly depart from the Markovian formula before ω/γ is as low as 5, χ has substantially departed from this already by $\omega/\gamma = 50$, one order of magnitude larger.

Let us now discuss the specific differences between the development in the exact solution and the Redfield limit. In 7.5(b) to 7.5(d) we see that the exact solution caries a notable oscillatory behavior that increases in strength when ω/γ decreases. This behavior is not shared by the Markovian approximation. This oscillatory behavior is however due to the specific interaction profile (W function) used in these plots, as is illustrated in 7.5(e) where a different W function is used.

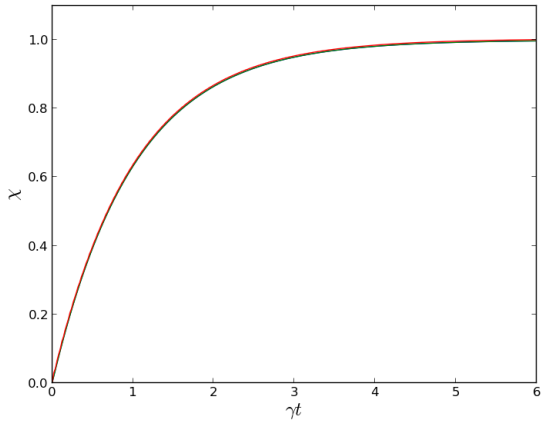
Another notable difference which applies in all cases, is that the limiting value of χ seems to increase as one moves away from the weak interaction limit. This also means that the oscillator settles at a higher temperature, which is weird since one would expect it to always settle at the initial temperature of the environment when the environment is large. A possible explanation of this lies in our choice to have the initial state of T bee on factorized form. When S and E are allowed to interact, they will depart from this initial factorization and entangle. This will release an additional interaction energy, which could heat up both the environment and the oscillator to a higher temperature. This effect would also increase with increasing interaction strength, just like we see to be the case in figure 7.5.

7.4.3 Decoherence in environments of finite size

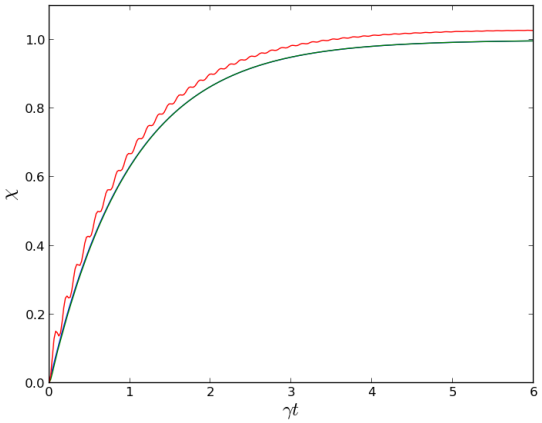
Finally, we will discuss the effects that moving away from the weak interaction limit has on decoherence, or more precisely the effects of having a finite environment. When one has a finite environment, that is a finite number of oscillators, the parameters r and χ will oscillate in some way over a characteristic period, as seen for instance in figure 7.5(f). This means that the coherence in the system will also return after some period. This is an effect which would be interesting to have a look at.

The remaining coherence between two coherent states $|z\rangle$ and $|w\rangle$ is still given by the formula 7.80. In the zero temperature case this depends only on r, and so it is clear that the coherences return precisely when the mechanical oscillations return to their initial amplitude. When the temperature is non zero however, also the temperature must return to its original value. This will make it harder for the coherences to return, as illustrated in figure 7.6.

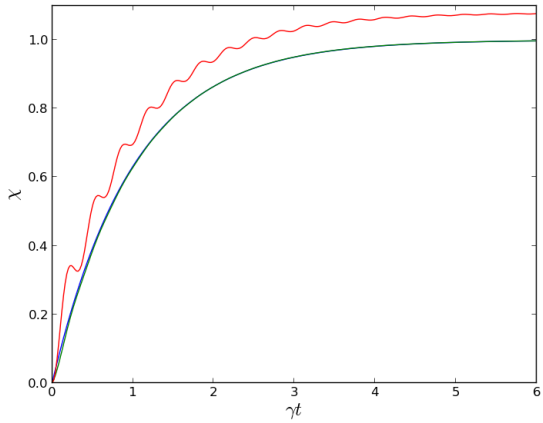
The figure shows how recurrences of coherence that are very distinct in the zero temperature case are damped out more and more at higher temperatures. It seems they can almost be completely removed, although one would need very high temperatures in order to do this. The reason for this damping is clearly the way that χ is present in expression 7.80. If χ is large, the effects of variations in r will be damped by a correspondingly large amount. Also, the higher the temperature is in the environment, the larger fraction of time will χ be large enough to make this damping substantial.



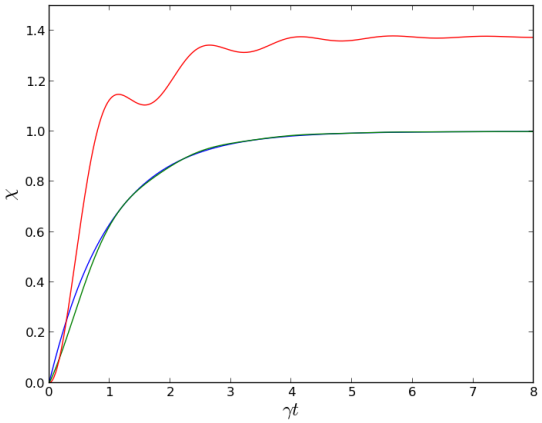
(a) $\omega/\gamma = 500$.



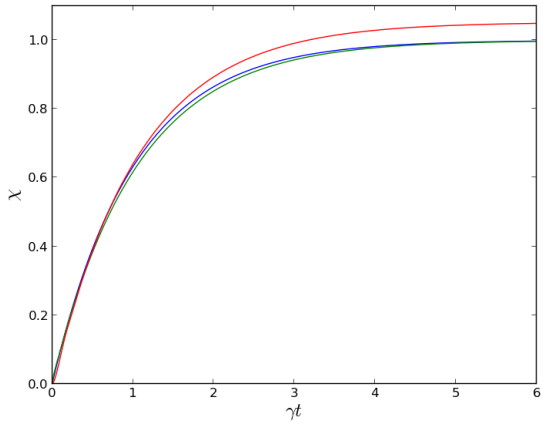
(b) $\omega/\gamma = 50$.



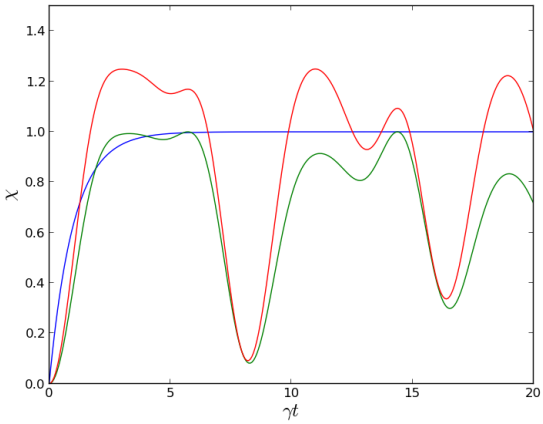
(c) $\omega/\gamma = 20$.



(d) $\omega/\gamma = 5$.



(e) $\omega/\gamma = 30$, linear W function.



(f) $\omega/\gamma = 2$, only three environmental oscillators.

Figure 7.5: Development of temperature describing parameter χ in the exact solution. The red curves show the actual behavior of the parameter, while the blue and green show the Markovian formula and its generalization respectively. In 7.5(a) the frequencies of the environmental oscillators are evenly distributed between 0 and 1000γ, while the interaction strengths are all the same. That is, the W function is flat. In 7.5(b) to 7.5(d) the frequencies are distributed between 0 and 200γ, while the W function is still flat. In 7.5(e) a linear W function has been used, whereas in 7.5(f) it is shown how χ behaves when the size of the environment gets extremely small.

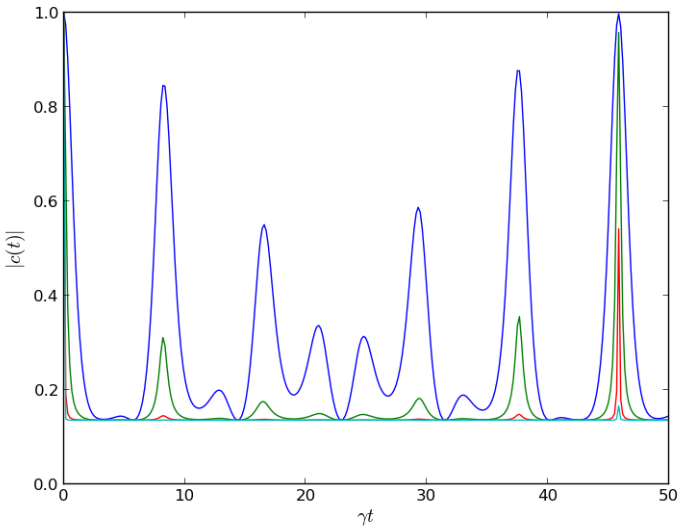


Figure 7.6: Effects of finite size on decoherence. Here the calculation is made with only three oscillators in the environment. The blue, green, red and cyan curves assumes temperatures of $\frac{k_B T}{\hbar\omega \ln 2} = 0, 5, 100$ and 2000 respectively. Note that the coherences that initially decay will return because of memory effects, but that these recurrences are strongly damped at high temperatures.

7.5 Summary of Conclusions

7.5.1 Concerning the system

The first conclusion we made concerning the behavior of this very simple model of an open harmonic oscillator is that the environmental coupling causes a damping of the oscillations. In the weakly interacting case this was a simple exponential damping on the form 7.34. In the more general case however we may have a more complicated damping. In fact we found that in general the complex parameter $r(t)$, which in a sense describes the orbit of the oscillator, is given by an expression that is completely analogous to that of the quantity $c(t)$ that was so extensively analyzed in the previous chapter.

In particular this means that the amplitude of the oscillations can have precisely the same evolution as $P(t)$ is shown to have in the figures of that chapter. Thus, if we move away from the weak interaction limit we may have a damping that looks like for instance the plots in figure 6.4. In addition, if we have an environment of finite size the damping will be reversed after a characteristic time, and the amplitude may take on an evolution of the type shown in for instance figure 6.3.

In addition to this we found that if the environment is in a state of finite temperature, then the oscillator will be heated by this. In the weakly interacting limit the temperature growth of the oscillator takes on the form shown in figure 7.3. Apart from a nearly instantaneous rise in temperature at $t = 0$, the curves are approximately described by Newtons law of heating and they approach the initial temperature of the environment. In the strongly interacting cases however, the temperature growth behaves in a much more complicated fashion, as seen in figure 7.5. Strictly speaking this figure shows the parameter χ which is the expectation value of the number operator of the translated oscillator, and thus related to the effective temperature.

A thing we noticed in particular was that these curves do not approach the initial temperature of the environment. We explained this by the fact that the oscillator S is initially in a state that is uncorrelated to the environment E, so that as correlations are formed there will be released an additional interaction energy which may be significant in the strongly interacting case. One may argue that this effect should be ignorable if the environment is truly large, since the released interaction energy must be distributed over all of this. One must however keep in mind that we by 'strongly interacting' here mean that we have

strong interactions with *each* of the environmental oscillators, so that the interaction energy will in fact scale with the size of the environment.

Another peculiar thing we notice about this model is that the mechanical damping and the heating of the oscillator are completely uncoupled: The expectation value $z(t)$ follows the same orbit in the complex plane irrespective of the temperature, and the temperature changes in the same way irrespective of the value of z. In particular, if the environment is initially in the vacuum state, then the temperature of the oscillator remains 0 no matter what happens to the mechanical degrees of freedom. This applies both in the weakly interacting limit and in the exact result.

This is a weird result since we would expect that in a realistic physical system friction would transfer some of the mechanical energy to heat, so that the damping of the oscillations should always be accompanied by an increase in temperature. It is however reasonable to expect that the lack off this effect is due to the simplicity of the model, and in particular the linearity of the interactions: If we had more general non-linear interactions, the ergodic hypothesis would cause us to believe that the individual degrees of freedom in the system should approach thermal states. This would effectively cause the environment to be heated by the mechanical energy transferred from the oscillator S, and this would again heat S.

In addition to the mechanical motion and the heating of the oscillator, we also analyzed the phenomenon known as decoherence. That is, the tendency of superpositions in certain bases to approach classical mixes of states from that basis. We found that both the energy basis and the coherent state basis to a degree can be said to have this character. That is, they are so called 'pointer bases', a nomenclature introduced by Zurek in [15]. This is because both of these bases were found to have the property that non-diagonal elements of the oscillator's density matrix were quickly damped when the indexes n and m or z and w were sufficiently far apart. More precisely we found that in the coherent state basis the non-diagonal elements fell off with a rate proportional to $|z-w|^2$. This rate was also found to be dependent on the temperature of the environment, as can be seen for instance in figure 7.4.

If the environment has a finite size, then just like the diagonal elements the non-diagonal ones will also return to their original value at sufficiently large times. In the zero temperature case this will happen over the same time scale as the mechanical evolution returns to its initial amplitude. This means that the original coherence returns to the system over this time scale, so that it can not be described classically over long time scales. However, if the environment is sufficiently hot, these recurrences will be strongly damped, as is seen in figure 7.6. Thus, even with a very small environment (in figure 7.6 for instance it only consists of three oscillators) the behavior of the system can still be thought of in classical terms as long as this environment has a sufficiently high temperature.

7.5.2 Concerning the methods

In this chapter I have only applied two different methods: The Redfield equation and an exact solution of the total system T. Let us first examine the degree to which the Redfield solutions are in agreement with the exact result: Well, first of all we note that these solutions are described by expressions that have the same form. That is, 7.97 has the same form as 7.33, while 7.112 has the same form as 7.65. The differences between the two are just the expressions for the parameters r and χ. In the Redfield result both of these have a simple exponential development, while in the exact solution $r(t)$ is the 00 component of the matrix $R = e^{-iWt/\hbar}$ and χ is given by the equation 7.111.

As I have mentioned, there is a complete correspondence between the parameter $r(t)$ from this chapter and the parameter $c(t)$ of the previous one. Since we concluded in the previous chapter that $c(t)$ has the form of a simple exponential decay in the limit of weak interactions and a continuous bath, we must conclude that the same holds true for $r(t)$. This parameter is thus in agreement with the Redfield result in this limit. That this is true also for the parameter χ can at least be seen to hold true in the example shown in figure 7.5. Our conclusion should thus be that the Redfield/Lindblad description is very good in the limit of weak interactions. This should really not be surprising, as this formalism was seen to be well justified in the first part of this thesis.

Let us finally say some words about the final method to be applied, namely the exact solution of T. Obviously this is the method that is the most believable (at least as long as one has sufficient faith in

ones ability to manipulate algebraic expressions). Also, if enormous accuracy is required or one is in a range of parameters where no approximation schemes works particularly well, this is of course the only method that can be applied. However, this method was found to be incredibly cumbersome and involved a great amount of work. In particular, a lot of this work came from the need to extract the relevant information about the reduced system S. This is something that we can definitely expect to generalize to more complicated models, if these can be solved exactly at all. We are thus forced to conclude that this approach does not generalize well.

Chapter 8

Discussion and future work

8.1 Review of discussions and conclusions

The purpose of this thesis has been to study the temporal development of open quantum systems. This involves both a question about what phenomenons will be encountered in such systems, a more general question about the form in which the time development can be written, and a question of which methods are useful when treating these systems. The most dramatic consequence of a system being open was derived already in section 3.1, where we found that unlike closed systems open systems will in general not develop unitarily: A pure state may develop into a mixed state. Thus, the time development postulate of quantum mechanics does not hold for open systems, and in particular such systems can not be described by a Schrödinger or Liouville equation. It thus becomes a central question whether there exists any general formalism that can replace this very useful description of quantum mechanical systems.

It was argued that the formalism for describing an open quantum system that is definitively the most general and believable, is to treat the system as being part of a larger composite quantum system T which is treated as closed. T then has a standard unitary development, and the development of our system S of interest can be found by taking the partial trace of the state of T. This approach has a clear advantage in that it only involves concepts and methodology that is well known and tested in the standard theory of closed systems. Also, in principle this approach allows models to be derived from first principles, which are always formulated in unitary terms.

For these reasons this subsystem description is very important from a theoretical point of view, but from a practical one the approach is not very useful: Even in such an extremely simple model as that of chapter 7 the process of reducing the description of the total system T to an effective description of S was found to be extremely cumbersome. It is thus desirable to have a formalism for time development which is more elegant, and which can be formulated in terms of the system S alone. In particular it is desirable to obtain a formalism which to a large degree is a generalization of the unitary time development postulate, and preferably also some sort of generalization of the Schrödinger/Liouville equations.

Such generalizations do exist, and there is an extensive literature devoted to them. An introduction is provided by my own main source, namely [2]. A major emphasis of this thesis has been that these approaches can be classified according to whether they are Markovian or non-Markovian. That is, whether the future development of S is determined using only information about its present state, or whether information about the past is also required. It is usually assumed that the development can be determined from the initial state, although I argued in section 3.3 that in general even this is a dubious assumption.

It is not hard to construct a heuristic argument for why open systems should in general be described in a non-Markovian fashion: Typically, information will leak from the system and into the environment. This information may return to the system at a later time and affect its development. If this information is only available in the environment, then the system can not be described in a Markovian manor. It is also easy to construct explicit examples of composite systems T where it can be proved that the reduced system S does not have a Markovian development. The only such explicit example to be included in this thesis is the one illustrated in figure 6.3, but one can construct examples that are much simpler than this.

The reader may choose to take this as an exercise.

However, as was argued in the discussions of the sections 4.2, 5.3 and 6.8, this generally non-Markovian character of open systems does not always show it self: Very often the system can be described using a Markovian formalism which is completely equivalent to the more general non-Markovian ones, and even to the subsystem description provided by 3.1. And even systems that can not be described in a Markovian manor like this at all times will *always* have such a description when the development is limited to a sufficiently short interval (at least when the system is finite dimensional). In section 4.2 I concluded that these exact Markovian descriptions are due to the invertibility of the time development operators (propagators).

Due to the difficulty of treating non-Markovian dynamics relative to Markovian dynamics it is thus reasonable to first attempt to use Markovian descriptions when dealing with some open quantum system. This will often work, and even when it does not the extra work put into the Markovian treatment is insignificant when compared to the work that will in any case have to be put into the non-Markovian one. Also, I suspect that manifestly non-Markovian behavior will typically only show itself in cases where it in any case is most interesting to include the part of the environment that causes this in the description of the system S itself. Even so, I will begin the review of these formalisms by discussing the Non-Markovian approaches.

8.1.1 Non-Markovian formalisms

The first reduced description of the time development of open systems that we encountered, was the Kraus decomposition 3.9. This is clearly a non-Markovian description, as it expresses the time development of the system in terms of the initial state. We thus have no guaranty that the later states can be found from the present one, nor indeed any other state except the initial.

The Kraus decomposition is a direct generalization of the unitary time development of a closed system: The difference is just that the time development operator U is replaced by a set of operators V_i. The development equation $\rho(t) = U\rho U^\dagger$ and the unitarity condition $U^\dagger U = I$ are replaced by the summation expressions 3.9 and 3.10. We found that a development on this form can be derived from a unitary model for the total system T consisting of S in combination with its environment, provided the assumption that the initial state factorizes. That is, the Kraus form 3.9 is implied by 3.2. We also found that the Kraus form is equivalent to certain more or less natural assumptions about the development of ρ, as described in theorem 1.

In section 3.3 I attempted to provide a discussion of whether these conditions are believable in general. It was easily seen that the conditions of trace preservation and complete positivity must hold in any meaningful development of a state operator. I thus concluded that it is really the condition of linearity, together with the assumption that the states at time t can at all be determined from the initial state that the Kraus condition hinges on. I remarked that these conditions are connected, as they are related to a need of regarding the environmental information as fixed in some way.

The only other non-Markovian description to be discussed significantly in this thesis, was the use of integro-differential equations: so called memory equations, which in general are on the form 5.1. In our discussions we however specialized this to linear memory equations, which are on the form 5.16. From a modeling perspective this description is clearly more useful than the Kraus form. When we are dealing with systems that have a truly non-Markovian character, such equations form the only possible generalizations of the Liouville/Schrödigenger equations used to describe unitary development: Attempting to describe the system using mere differential equations always results in Markovian behavior.

The memory equation approach was found to be particularly useful in our treatment of the model in chapter 6, where we saw that this system can be described exactly by such an equation, and that this is scalar and has an exactly calculable kernel. This was equation 6.36, with the kernel $K(t-t')$ given by 6.34. This equation was found to be very powerful in the analysis of that model: We could use it to show that we have exponential decay in the weak interaction or 'Markovian' limit, we could use it to analyze under what conditions the decay will be exponential asymptotically, and we could also use it to understand the strongly non-Markovian consequences of having an environment of finite size.

Although the use of memory equations thus seem to be a powerful approach, when dealing with more general models we can neither expect them to be scalar nor to have an exactly calculable kernel: The only memory equation I know to describe open systems in general is the Nakajima Zwanzieg equation 5.4, where the kernel is a superoperator and must in general be expanded using 5.14. The Nakajima Zwanzieg equation is equivalent to and can be derived from a unitary model of $T = S \cup E$. The version of the equation that was discussed in this thesis assumes that the initial state of T factorizes. The equation can however be generalized to arbitrary initial conditions at the cost of loosing linearity[2]. Note that this would imply that the development can not be written in Kraus form.

In this thesis the only direct application of the Nakajima Zwanzieg equation was in section 6.7. We there remarked that the results shown in figure 6.12 seem to indicate that the solutions of the Nakajima Zwanzieg equation converges towards the solution of the scalar memory equation when the order of the kernel expansion is increased. We however also saw that the calculation of these expansions can be assumed to be an extraordinarily laborious task.

8.1.2 Markovian formalisms

Let us now turn to the Markovian formalisms for describing open systems: The most general Markovian generalization of the unitary time development postulate for open systems is clearly 4.1. This is however to general, in that we have no way of guaranteeing that this describes a meaningful evolution of a state operator. This is improved upon by assuming that the operators $\mathcal{G}(t, t')$ are trace preserving and completely positive, in which case the evolution can be written as 4.3 and is referred to as a quantum dynamical semigroup.

This is in a way a more direct generalization of the unitary cases: it is simply a generalization of the Kraus decomposition to an expression involving any earlier time instead of just the initial one. However, unlike the unitary case where $|\psi(t)\rangle = U(t, t')\,|\psi(t')\rangle$ is equivalent to $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$, a description in terms of quantum dynamical semigroups is not equivalent to Kraus decomposition. Also, assuming that the operators $\mathcal{G}(t, t')$ form a quantum dynamical semigroup will cause a lack of generality, since not all meaningful Markovian developments of state operators are described by such groups: This is because these operators need not necessarily be positive when $t' \neq 0$.

The generalizations of the Liouville/Schrödinger equations will in the Markovian framework obviously be much closer to these equations themselves, in that they will be differential equations rather than integro differential equations. The most general such equation is clearly 4.6, but again this is really to general: here too we can not guarantee a meaningful development of the state operators. This can however be solved by taking the Markovian generator $\mathcal{M}_t$ to be the one defined in 5.17, which gives the *exact* Markovian description of the system, provided of course that such a description exists. This generator is in general not exactly calculable, and it must typically be expanded as 5.25. The contributions up to the sixth order are found in the equations 5.36 to 5.40.

The lowest order of this expansion gives rise to the Redfield equation, 4.29 or 4.30. Using 4.30 is the simplest way to derive an approximate Markovian description of S from a unitary model of the total system $T = S \cup E$. This approximation is good when the interactions between S and E are weak, or equivalently when there is time scale separation of the type described in section 5.2 and much of chapter 6. In both chapter 6 and 7 we compared the results of the Redfield equation with exact solutions, and we saw the correspondence to be excellent in this limit.

The strict condition for the Redfield equation to apply is that the interaction strength must be weak when compared to a energy scale in the environment. If we also assume that the interaction strength is weak when compared to a scale in the system, then the Redfield equation can be written in Lindblad form[2]. The Lindblad equation 4.8 or 4.9 is the differential equation corresponding to the quantum dynamical semigroup 4.3, from which it can also be derived. This was done in the main text. The Lindblad equation also always describes meaningful developments of state operators. In addition it can be seen to have the form of a very direct generalization of the Liouville equation, and it is expressed in terms of objects that have simple physical interpretations. For these two reasons it is clearly very useful

for modeling purposes. In fact, as long as the interactions are not to strong, the Lindblad equation seems to always be a good alternative for a first attempt of modeling an open system.

A Markovian expansion of the form described above can in fact be derived from any memory equation of the type 5.16. The general expansion is given by equation 5.24. In particular, in section 6.8 we used this to derive an expansion of the Markovian generator corresponding to the scalar memory equation 6.36. The solutions to the resulting differential equation was compared to the solutions of the memory equation itself. Provided we went to a sufficiently high order in the expansion the agreement was in most cases found to be excellent even for quite strong interactions.

8.1.3 Additional

Let us end the review of conclusions by making some simple remarks about what the two very simple models studied in this thesis can tell us about the general behavior of open systems: In the first model, as noted in that chapter, the only consequences that could be seen was that the coupling to the environment caused an effective energy shift, and also incoherent transfers to a state of lower energy: That is, the system looses energy to the environment. The shift of energy is something we can expect to always generalize to other systems, while the loss of energy will obviously only occur if the environment has an effectively lower concentration of energy than the system. This was for instance seen to be the case in the second model, where the mechanical motion of the oscillator was always damped, whereas the temperature approached that of the environment: Thus, if the oscillator was initially prepared in a state of lower temperature, then the flow energy would go from the environment to the oscillator.

Concerning the decay of the two level model, we found that in the limit of weak interactions the decay will be exponential over the period where most of this decay occurs. For very short times we found that in rigorous quantum mechanical models the decay must proceed quadratically. The time scale over which this is the case is however inversely proportional to the energy range in the environment to which the system interacts. For realistic physical decays this can typically be assumed to be an extremely short time scale. Both the seemingly exponential form of decaying levels and the initially quadratic one is something we can expect to generalize to other models.

We also found that the two level model deviates from exponential decay for very large times. Whether this is something that generalizes to more realistic models is more questionable: In a more realistic model we would expect decoherence to cause a transition to classical behavior over very long time scales. Classically the system is described by probabilities alone, and the development must thus proceed exponentially as long as it is memoryless. On the other hand this is of course not necessarily the case, although it is a natural assumption due to the extreme dilution of information that will eventually happen when the system is coupled to the universe at large.

The mechanical damping of the oscillator is also something we would expect to generalize to other systems: Although energy may as mentioned flow from the environment and to the oscillator, this will almost always be in the form of chaotic thermal energy, and not in the form of ordered mechanical motion. Such ordered motion we can typically assume to be absorbed by the environment and converted to heat. This does in fact not take placed in the simple model employed in this thesis: the damping of the oscillator is not coupled to the temperature development at all. As mentioned in that chapter I expect that this is due to the linearity of the interactions.

Finally, let us turn to the very interesting phenomenon of decoherence, which as mentioned is a subject I have been able to devote far less space to than I would have wanted. Here decoherence should be interpreted not merely as the transition from pure to mixed states, but as specifically the tendency of non-diagonal elements of the state matrix to be quickly damped in some basis. We saw that in the harmonic oscillator model the state matrix seemed to have this character both when expressed in the number and coherent state bases. That is, these bases are so called pointer bases [15].

In the two level model we saw no signs of decoherence in this sense. This is definitely not something that should be expected to be a realistic trait of that model, as indeed the fact that such decoherence takes place over a time scale that is faster than the mere decay is well known both in the theory and experiments of NMR[1]. In the oscillator model, the non-diagonal elements did fall of over a time scale

that was faster than the 'physical' evolution in the mentioned bases, but only when these elements were far from the diagonal. In addition the rate of decoherence was found to increase with temperature. Both of these traits are something we expect to generalize to at least some more realistic models.

8.2 Future work

As often is the case when one suddenly has to put a great amount of work into a field one has never before encountered, the work with this thesis has brought up more questions than it has answered. Indeed, most of these questions are much more interesting than the conclusions that have actually come out of the thesis. Many of them can probably be answered by diving deeper into the literature than I have been able to do during my work, but some of them it could also be fun to attempt to answer by generalizing the treatments I provide in the thesis. I would have liked to try to answer some of these questions, but as a master thesis is something that must be finished within a fixed amount of time, this is not something I could include here. And to be honest I am glad for this, as I am at the present time looking forward to having some spare time again. In any case I include in this section a list of some work that could have been done in an extend version of this thesis.

8.2.1 Concerning the two level model

The most interesting question that remains unanswered in connection to the two level model, is connected to the asymptotic behavior of the decay. In sections 6.6.3, 6.6.6 and 6.8 we obtained strong indications that the decay is asymptotically exponential (that is, it has an asymptotic decay rate) as long as the memory kernel is exponentially bounded (plus some additional integral conditions). Even so, I have provided no proof of this. It would be interesting to see if some such proof can be constructed, and I strongly suspect that this is possible by using the expansion of section 6.8:

It is in fact not very difficult to show that under appropriate conditions the individual contributions of this expansion has a well defined limit when $t \to \infty$. Thus all one needs to do is to show that the sum of all these limits is well defined and finite. Some additional conditions might be needed for this. Also, one would obviously have to prove that the generator 6.84 indeed does describe the decay exactly. This would among other things involve proving that the development operators $\mathcal{G}_t$ are invertible, as discussed in section 4.2.

Another question that is connected to this is precisely what the exponential bounding of the memory kernel means in terms of the W function. That is, can this condition be expressed in terms of some condition involving $W(\omega)$ rather than its Fourier transform? [13][6] claims that if the W function is non-zero only in a semifinite interval, then the decay must asymptotically proceed as a power law instead of exponentially. Another thing that would be interesting to examine is whether this asymptotic power law behavior is something that can be understood using the memory equation approach.

An additional thing that could have been included in the two level chapter, is a Markovian treatment using the expansion 5.25. Also, I could have attempted to computer automate the expansion of the Nakajima Zwanzieg kernel, so that this could have been taken to a higher order than four. This would not have given any additional physical insights, but it could have demonstrated whether these expansions are in agreement with the other methods as they are supposed to.

8.2.2 Concerning the harmonic oscillator model

The major questions of interest concerning the harmonic oscillator model, are connected to the consequences of incorporating more general interactions. This includes both the consequences of including more general linear interactions, and also the consequences of having nonlinear interactions between the oscillators. Let us first discuss the questions connected to generalizing the linear interactions: As mentioned at the beginning of chapter 7 this is a question that is treated other places [2][3]. There is however one question in connection to this that does not emerge in clarity from these sources.

One of the most striking features of the model employed here is that as long the environment is in the vacuum state, then pure coherent states of S remain such pure coherent states through their development. Note that this was a feature not only of the weak interaction limit, but also of the exact solution. It would be interesting to see whether this in some way is something that generalizes to more general interactions. That is, we might wonder whether there also in these cases exists states that remain pure through their development.

Actually it is not very hard to see that this can not be the case: with more general interactions even the ground state would be correlated with the environment, and the reduced state would be mixed. As it is reasonable to expect that any state will be damped so as to end up in this ground state, it can not remain pure through its entire development. Even so it would be interesting to see how this conservation of purity best generalizes to more general interactions. This is clearly connected to Zurek's pointer basis concept.

In connection to including non linear interactions, I discussed one possible consequence of this already in the main text: In our simple linear model the mechanical and thermal evolutions were completely uncoupled. In particular the mechanical damping did not cause a heating of the system, as we would expect in a physically realistic oscillator that is damped by friction. This is something I would expect to generalize to other linear models, as linear interactions have no way of converting the ordered mechanical motion in to chaotic heat. If we include non-linear interactions however, this motion might take on a sufficiently chaotic character to be be simlar to heat. It thus becomes an interesting question whether including such non-linear interactions in the model might reproduce the effects of heating by friction.

I also suspect that to include non-linear interactions might have some consequences for the decoherence: Possibly this could lead to non-diagonal elements being quickly damped also when they are close to the diagonal. After all, this is something that does happen in realistic physical systems, such as the NMR case for instance. Also, I wonder whether non-linear interactions might cause the recurrences of coherence shown in figure 7.6 to occur after much longer time scales. This is because non-linear interactions would allow the environment to make use of a much larger fraction of its phase space, thus decreasing the probability of overlap between states (See equation 7.91).

In general decoherence and pointer basis states is something i find very interesting and would like to study in more detail.

8.2.3 Concerning the general theory

In connection to the general theory of time development in open systems, there is particularly one question that has not been answered in a completely satisfactory manor. This is in connection to the conditions for Kraus decomposition, where the conditions of linearity and determination from the initial state could not be defended in a completely general manor. We found however that these conditions follow if we assume that the initial state of T is a function of the initial state of S. That is, if $\rho_T = \mathcal{L}\rho_S$. The map $\mathcal{L}$ must be linear. In addition it must clearly be trace preserving, completely positive and have the property that $\mathrm{Tr}_E \mathcal{L}A = A$.

The only example of such a function given in the main text was the trivial case of factorizing initial conditions, where $\mathcal{L}A = A \otimes \rho_E(0)$. A question that is very interesting is if one can find a function of this type which describes a more realistic situation than factorizing initial conditions. I commented in the main text that it is difficult to find examples of such functions at all, but I will now in fact attempt to construct one that I find physically meaningful:

Assume that the total system T starts out in a factorized state $\rho_T(0) = \rho_S(0) \otimes \rho_E(0)$, and that the reduced system S has a time development which is invertible. That is, the time development operators $\mathcal{G}_t$ have left inverses $\mathcal{G}_t^{-1}$. Then we may construct maps that we could denote $\mathcal{L}_t$ by the relations

$$\mathcal{L}_t A = U(t)\left(\left(\mathcal{G}_t^{-1}A\right) \otimes \rho_E(0)\right) U(t)^\dagger. \tag{8.1}$$

These maps take the state of S at time t to the state of T at time t. They are clearly linear, trace preserving and have the property that $\mathrm{Tr}_E \mathcal{L}_t A = A$.

Whether they are completely positive is however more dubious. This is for the same reasons as was explained in conection to general Markovian development in section 4.1: As $\mathcal{L}_t$ takes state operators of S to state operators of T, any *allowed* state must go to a positive operator. However, we do not actually have any guarantee that all states are allowed at time t, and thus all positive states need not go to positive states. If however such an operator can be shown to be completely positive, then it gives us a way of fixing the environmental information by demanding that $\rho_T(0) = \mathcal{L}_t\rho_S(0)$.

Also, this particular way would imply that the Kraus conditions are satisfied. The operators $\mathcal{L}_t$ are particularly interesting if they have a nontrivial limit when $t \to \infty$. This could for instance be denoted $\mathcal{L}_\infty$. Choosing any particular value for t in this set of operators is in a way just as arbitrary as choosing $t = 0$, which corresponds to factorizing initial conditions. $\mathcal{L}_\infty$ however, would not be an arbitrary choice: this would correspond to a system having formed precisely those correlations with its environment that they in any case would form if left alone for a while. I would even say that in general these are in fact the most believable initial conditions.

This is a subject I have devoted a small amount of thought to, and it would be interesting to examine these questions in more detail. This will however not be done in this thesis, which the reader has now finished.

Appendix A

Computer codes

In the models studied in this thesis, numerical calculations of various types have been employed. These have been implemented as Python scripts, which I have run on my own computer. In case the reader wishes to have a look at some of theese concrete implementations, I include all my scripts in this apendix.

A.1 Two level decay diagonalization code

The following is the Python script used to diagonalize the model of two level decay:

```
#Importing libraries that may be needed
import numpy as np
import numpy.linalg as la
import matplotlib.pyplot as pp
import scipy.optimize as op
import cmath as cm
import scipy.integrate as ig


#Parameters

T=14.          #Time interval where c(t) is calculated
res=200        #Resolution of plot

E=5.0          #Energy of exited state
deltaE=80      #characteristic energy range parameter
Erad=5*deltaE #Radius of energy range in the environment in which oscillators are placed

dec=1.0        #1. order perturbation theory decay rate

n_osc=500      #number of oscillators in environment

p=0.1          #Anti-symmetry parameter

#W-function definitions

f1=lambda x: (np.abs(x)<=deltaE)*(1+p*x)        #FLat/Linnear
f2=lambda x: np.exp(-x*x/(2*deltaE*deltaE))     #Gaussian
f3=lambda x: np.exp(-np.abs(x)/deltaE)          #Exponential
f4=lambda x: 1.0/(1.0+x*x/(deltaE*deltaE))      #Lorenzian

f=lambda x:(1.0/2/np.pi)*f2(x)                  #W-function type is chosen here


#Initialization of environmental information

frq_start=E-Erad                                #Start of environmental frequency range
```

```
frq_stop=E+Erad                                  #End   of environmental frequency range

frq=np.linspace(frq_start,frq_stop,n_osc)  #All frequencies
cpl=np.sqrt(f(frq))                              #All interaction parameters (w_i)

dim=1+n_osc                                      #Dimension of Hilbert space


#Initialization of Hamiltonian

H=np.zeros([dim,dim])                #Hamiltonian matrix
H[0,0]=E                             #Energy of state |e)
for i in np.arange(0,n_osc):
        H[i+1,i+1]=frq[i]            #Energy of state |i)
        H[0,i+1]=H[i+1,0]=cpl[i]     #Interaction between |e) and |i)


#Calculation

w, v = la.eig(H)                         #Diagonalizes H, w is eigenvalues and v is
    transformation matrix
u0=np.zeros(dim)                         #Vectorial representation of initial state
u0[0]=1                                  #Initial state = |e)
vt=np.swapaxes(v,0,1)                    #Adjoint of transformation matrix
v0=np.dot(vt,u0)                         #Initial state in diagonalized basis

def u(t):                                #Returns state at time t
        mv=v0*np.exp(-1j*t*w)            #State at time t in diagonalized basis
        return np.dot(v,mv)              #State at time t in original basis

def du(t):                               #Returns derivative of u
        mv=-1j*w*v0*np.exp(-1j*t*w)      #Derivative in diagonalized basis
        return np.dot(v,mv)              #Derivative in original basis

def p1(t):                               #Returns c(t) = amplitude for being in state |e)
        return (u(t))[0]

def dp1(t):                              #Returns derivative of c(t)
        return (du(t))[0]

#Plotting

x=np.linspace(0,T,res)                   #Time interval to plot
y=1j*np.zeros(x.size)                    #Values
for i in np.arange(0,res):
        y[i]=np.abs(p1(x[i]))**2         #Probability for being in state |e) at time t

#pp.plot(x[0:res],y[0:res].real)         #Plot real      part of c(t)
#pp.plot(x[0:res],-y[0:res].imag+E)      #Plot imaginary part of c(t)

pp.plot(x,y)                             #Plot P(t)

pp.xlim(0,T)                             #Limits
pp.ylim(0,1)
pp.show()                                #Draw results
```

A.2 Assymptotic decay-rate plot-code

This is the code used to display the graphs and simmulation points in figure 6.11:

```
#Importing libraries that may be needed
```

```
import numpy as np
import scipy.optimize as op
import scipy.special as spes
import matplotlib.pyplot as pp

#Data arrays containing assymptotic decay rates from simmulations

#Results from gaussian W-function  simmulation
RATE = np.array([1.005,1.006,1.007,1.010,1.021,1.043,1.093,1.174,1.328,1.402])
DW=np.array([100,80,60,40,20,10,5,3,2,1.8])     #Delta-E parameter

#Results from lorenzian W-function simmulation
RATE2 = np.array([1.005,1.006,1.009,1.013,1.026,1.056,1.13,1.267,1.581])
DW2=np.array([100,80,60,40,20,10,5,3,2.15])     #Delta-E parameter


#Equation solver to find Gaussian result

#Equation to be solved is
#Gamma/Gamma_pt = exp( Gamma^2/8 Deltaomega^2 ) * ( 1 + erf( Gamma/sqrt 8 Deltaomega ) )

#Defining x       = Gamma/Gamma_pt,
#         w(x)    = x/(sqrt 8 Deltaomega/Gamma_pt)  and
#         f(x) = x - exp( w^2 ) * ( 1 + erf( w ) )

#This can be written simply as f(x)=0

def f(x,w):                                     #Definition of f
        return x-np.exp(w*w)*(1+spes.erf(w))    #As above

def find(x,k):                          #Finds solution to f(x)=0 for vector of x
        n=len(x)                        #Length of vector
        prev=k                          #Initial guess
        y=np.zeros(n)                   #Vector of solutions
        for i in np.arange(0,n):
                prev=y[i]=op.newton(lambda z: f(z,z*x[i]/np.sqrt(8.0)),prev, tol=1e-10)
        return y                        #Solution is found through Newtons method



#Analytic results

x=np.linspace(0.0,0.6,200)  #Range of Gamma_pt / Delta omega
y=find(x,1)                 #Gaussian Result
y2=(1-np.sqrt(1-2*x))/x     #Lorenzian result
y2[0]=1.                    #Limit

#Ploting

pp.plot(x,y)                                                    #Plot Gaussian  analytic result
pp.plot(x,y2)                                                   #Plot Lorenzian analytic result
pp.xlim(0,0.6)                                                  #X-limits small version
pp.ylim(1,1.8)                                                  #Y-limits big version
pp.xlabel("$\Gamma_{pt}/\Delta\omega$",fontsize=18)             #X-axis label
pp.ylabel("$\Gamma/\Gamma_{pt}$",fontsize=18)                   #Y-axis label
pp.plot(1.0/DW,RATE,marker='o',linestyle='')                    #Plot Gaussian  simmulation result
pp.plot(1.0/DW2,RATE2,marker='*',linestyle='')                  #Plot Lorenzian simmulation result
#pp.xlim(0,0.06)                                                #X-limits small version
#pp.ylim(1.,1.03)                                               #Y-limits small version

pp.show()                                                       #Draw results
```

A.3 Long range Decay-rate code

The following code finds the long range behaviour of the decay rate by solving the memory equation for $c(t)$, and differentiating this numerically:

```
#Importing libraries that may be needed
import matplotlib.pyplot as pp
import memeq
import numpy as np
import numpy.linalg as la

#Parameters

Wrad=80             #Characteristic energy range parameter

nder=20             #Number of displacement steps used in numerical differentiation

Erad=1000*Wrad      #Total range of frequencies
npoints=10000000    #Number of frequency samples

res=5000            #Plot resolution
T=14                #Time interval to be plotted

#W-function definitions

f1=lambda x: np.abs(x)<=Wrad                #FLat
f2=lambda x: np.exp(-x*x/(2*Wrad*Wrad))     #Gaussian
f3=lambda x: np.exp(-np.abs(x)/Wrad)        #Exponential
f4=lambda x: 1.0/(1.0+x*x/(Wrad*Wrad))      #Lorenzian

f=lambda x:(1.0/2/np.pi)*f2(x)              #W-function type is chosen here

#Initialization

Pp=int(2*Erad/Wrad)                                 #Length of periodic averages
npp=npoints/Pp                                      #Number of periodic averages

E_spacing=2*Erad/npoints                            #Distance between frequency samples

Tmax=np.pi*npoints/Erad                             #Total time interval

E=np.linspace(-Erad,Erad-E_spacing,npoints)         #Frequency  samples
W=f(E)                                              #W-function samples

#calculation

K,y=memeq.decay(W,2*Erad,2*E_spacing)                           #Gets c(t)
y=np.abs(y)**2                                                  #     P(t)

yd=(y[nder:npoints]/y[0:npoints-nder]-1)*Erad/np.pi/nder        #Numerical logaritmic
    derivative

myd=np.ones(npp)                                                #periodic averages
for i in np.arange(0,npp):
        myd[i]=np.mean(yd[Pp*i:Pp*(i+1)])                       #i'th average

xpp=np.arange(0,npp)*2*np.pi/Wrad+np.pi/Wrad                    #Medium positions of average
    ranges

#Plotting

#Plots logaritmic derivative
```

```
pp.plot(np.linspace(0,Tmax-(1+2*nder)*Tmax/npoints,npoints-nder),-yd[0:npoints-nder])
#pp.plot(xpp,-myd, linestyle="",marker='.')  #plots periodic averages

pp.ylabel("$-\dot P/P$",fontsize=18)          #Y-axis label
pp.xlabel("$\Gamma_{pt}t$",fontsize=18)       #X-axis label
pp.ylim(0.4,1.4)                              #Limits
pp.xlim(0,T)
pp.show()                                     #Draw results
```

A.4 Library for solving memory equations

The following code is a library used to solve memory equations numerically. This is done by first calculating the Laplace transform of the Kernel, and then the Laplace transform of the solution $c(t)$ throught the formula 6.63. The solution it self is the found by taking the inverse Laplace transform of this result. This is done by use of the Mellin formula, which can be written as $e^{\lambda t}\mathcal{F}^{-1}(a(i\omega+\lambda))$. $\mathcal{F}^{-1}$ is the inverse Fourier transform.

```
#Importing libraries that may be needed
import numpy as np
import scipy.fftpack as ftp
import matplotlib.pyplot as pp



#Function decay finds probability amplitude c(t) for a decaying two level system given
    the
#W-function. The frequency range D and a Lambda parameter used in the mellin formula
#must be specified.
def decay(W,D,Lambda):
        n=len(W)                              #Vector length
        K=-ftp.fft(W)*D/n                     #Memory kernel, given by the fourier transform
            of W
        y=1-2*(np.arange(n)%2)                #Rapid oscillations
        K=K*y                                 #must be divided out of K to compensate for the
             fact
                                              #that the FFT algorithm assumes that negative
                                              #frequencies are in the last part of the input
        K[n/2:n]=np.zeros(n/2)                #Negative frequencies are eliminated
        T=2*np.pi*n/D                         #Total time interval
        return K, solMemeq(K,T,Lambda)        #Returns memory kernel and solution c(t)


#Function solMemeq solves a memory equation given a memory kernel x. The time interval T
    and a
#Lambda parameter used in the mellin formula must be specified. It is assumed that c(0)=1
def solMemeq(x,T,Lambda):
        n=len(x)                              #Vector length
        S=2*np.pi*n/T                         #Laplace transformed interval
        s=1j*np.linspace(0,S-S/n,n)           #Laplace transformed variable
        s[n/2:n]=s[n/2:n]-1j*S                #negative values
        s=s+Lambda                            #Shift by lambda specified by mellin formula
        y=flt(x,T,Lambda)                     #Laplace transform of kernel
        y=1/(s-y)                             #Laplace transform of solution
        return ilt(y,T,Lambda)                #returns solution, found by inverse laplace
            transform


#Function flt calculates the laplace transform of x along a line in the imaginary
    direction.
#The time interval T and the Real coordinate Lambda of the line must be specified.
```

```
def flt(x,T,Lambda):
        n=len(x)                          #Vector length
        t=np.linspace(0,T-T/n,n)          #samples of t
        t[n/2:n]=t[n/2:n]-T               #negative values
        y=np.exp(-Lambda*t)*x             #Exponential of the real part of s
        return ftp.fft(y)*T/n             #Laplace transform calculated through FFT
            algortihm


#Function ilt calculates the inverse laplace transform of x. The time interval T and  a
    Lambda
#parameter used in the mellin formula must be specified.
def ilt(x,T,Lambda):
        n=len(x)                          #Vector length
        y=ftp.ifft(x)*n/T                 #Inverse fourier transform calculated through
            IFFT
        t=np.linspace(0,T-T/n,n)          #samples of t
        t[n/2:n]=t[n/2:n]-T               #negative values
        return np.exp(Lambda*t)*y         #Inverse Laplace given by Mellin formula
```

A.5 Memory equation solver of Nakajima Zwanzieg kernel

This code is used comparing the functions $P(t)$ found from solving 2. and 4. order approximations to the Nakajima Zwanzieg equation, to those found from solving the exaxact memory equation described in section 6.6.

```
#Importing libraries that may be needed
import matplotlib.pyplot as pp
import memeq
import numpy as np
import numpy.linalg as la
import scipy.fftpack as ftp
import scipy.signal as sig


#Parameters

Wrad=2              #Characteristic energy range parameter

Erad=1000*Wrad      #Total range of frequencies
npoints=1000000     #Number of frequency samples

res=5000            #Plot resolution
T=3.                #Time interval to be plotted
samp=1              #Fraction of samples to be plotted

#W-function definitions

f1=lambda x: np.abs(x)<=Wrad                #FLat
f2=lambda x: np.exp(-x*x/(2*Wrad*Wrad))     #Gaussian
f3=lambda x: np.exp(-np.abs(x)/Wrad)        #Exponential
f4=lambda x: 1.0/(1.0+x*x/(Wrad*Wrad))      #Lorenzian

f=lambda x:(1.0/2/np.pi)*f1(x)              #W-function type is chosen here

#Initialization

E_spacing=2*Erad/npoints                    #Distance between frequency samples

E=np.linspace(-Erad,Erad-E_spacing,npoints)  #Frequency  samples
```

```
W=f(E)                                          #W-function samples
Tmax=np.pi*npoints/Erad                         #Total time interval

#calculation

K,y=memeq.decay(W,2*Erad,2*E_spacing)           #Gets memory kernel K and c(t)

nshow=int(npoints*T/Tmax)                       #Number of samples shown in plot
t=np.linspace(0,(nshow-1)*Tmax/(npoints-1),nshow) #Time samples

K1=np.cumsum(K)*Tmax/(npoints-1)                #Cumulative integral of K
K2=np.cumsum(K1)*Tmax/(npoints-1)               #Cumulative second integral of K

#Convolution of K*K1 of K and K1. Calculated in Fourier domain for efficiency
KC1=sig.fftconvolve(K,K1)[0:npoints]*Tmax/(npoints-1)

KO4=K*(1+K2)-KC1+abs(K1)**2             #4.order aproximation to memory kernel

#P(t) found by solving 2. order memory equation
y2=memeq.solMemeq(2*K.real,Tmax,2*E_spacing)

#P(t) found by solving 4. order memory equation
y4=memeq.solMemeq(2*KO4.real,Tmax,2*E_spacing)

#Plotting

pp.plot(t[::samp],abs(y[0:nshow:samp])**2)  #Plot exact P(t)
pp.plot(t[::samp],y2[0:nshow:samp])         #Plot 2. order approximation
pp.plot(t[::samp],y4[0:nshow:samp])         #Plot 4. order approximation

pp.xlim(0,T)                                #Limits
pp.ylim(0.,1.)
pp.xlabel("$\Gamma_{pt}t$",fontsize=18)     #Labels
pp.ylabel("$P$",fontsize=18)
pp.show()                                   #Draw results
```

A.6 Code for calculating n'th order scalar Markovian generator

This code calculates and plots the Markovian generators of different orders that aproximate the scalar memory equation described in section 6.6. This is done following the procedure described in section 6.8.

```
#Importing libraries that may be needed
import matplotlib.pyplot as pp
import memeq
import numpy as np
import numpy.linalg as la
import scipy.fftpack as ftp
import scipy.signal as sig


#Parameters

Wrad=10.            #Characteristic energy range parameter

order=9             #Number of orders to be included

Erad=1000*Wrad      #Total range of frequencies
npoints=1000000     #Number of frequency samples

res=5000            #Plot resolution
T=10                #Time interval to be plotted
```

```
samp=1              #Fraction of samples to be plotted
nder=10             #Number of displacement steps used in numerical differentiation

#W-function definitions

f1=lambda x: np.abs(x)<=Wrad                #FLat
f2=lambda x: np.exp(-x*x/(2*Wrad*Wrad))     #Gaussian
f3=lambda x: np.exp(-np.abs(x)/Wrad)        #Exponential
f4=lambda x: 1.0/(1.0+x*x/(Wrad*Wrad))      #Lorenzian

f=lambda x:(1.0/2/np.pi)*f1(x)              #W-function type is chosen here

#Initializatoion

E_spacing=2*Erad/npoints                                #Distance between frequency samples

E=np.linspace(-Erad,Erad-E_spacing,npoints)             #Frequency  samples

W=f(E)                                                  #W-function samples
Tmax=np.pi*npoints/Erad                                 #Total time interval

#Calculation

K,y=memeq.decay(W,2*Erad,2*E_spacing)                   #Gets memory kernel K and c(t)

nshow=int(npoints*T/Tmax)                               #Number of samples shown in plot
t=np.linspace(0,(nshow-1)*Tmax/(npoints-1),nshow)       #Time samples

y=np.abs(y)**2                                                  #Exact probability P(t)
yd=(y[nder:npoints]/y[0:npoints-nder]-1)*Erad/np.pi/nder         #Numerical logaritmic
    derivative of P(t)
#pp.plot(t[::samp],d[0:nshow:samp])                             #Plot P(t)
pp.plot(t[::samp],-yd[0:nshow:samp])                            #Plot exact instantaneous
    decay rate

K1=np.cumsum(K)*Tmax/(npoints-1)        #Cumulative integral of K
K2=np.cumsum(K1)*Tmax/(npoints-1)       #Cumulative second integral of K
msub=[K1]                               #Definition of  m_0
mupp=[K1]                               #Definition of  l_0
mbar=[K2]                               #Definition of _l_0


#Contributions of order n to the markovian generator are calculated following the
    reccursive procedure described in the text.
for n in np.arange(order-1):
        q=np.cumsum(mupp[n])*Tmax/(npoints-1)
        q=sig.fftconvolve(K,q)[0:npoints]*Tmax/(npoints-1)
        mupp.append(q.copy())
        q2=np.cumsum(q)*Tmax/(npoints-1)
        for j in np.arange(n+1):
                q-=mupp[n-j]*mbar[j]
                q2-=np.cumsum(mupp[n-j])*Tmax/(npoints-1)*mbar[j]
        mbar.append(q2.copy())
        msub.append(q.copy())


#Plotting

mtot=0 #Total markovian generator
for n in np.arange(order):
        mtot+=msub[n]                           #n'th order contribution
        q=np.cumsum(mtot)*Tmax/(npoints-1)      #Integral of generator
        q=np.exp(2*q.real)                      #P = |c|^2 = |exp q|^2
```

```
        pp.plot(t[::samp],-2*(mtot[0:nshow:samp]).real)  #Plot n'th order generator
        #pp.plot(t[::samp],q[0:nshow:samp])               #Plot P(t)


pp.xlim(0,T)                                    #Limits
pp.ylim(0.,2.0)
pp.xlabel("$\Gamma_{pt} t$",fontsize=18)        #Labels
pp.ylabel("$-\dot P/P$",fontsize=18)
pp.show()                                       #Draw results
```

A.7 Code for plotting n-basis density matrix

This code calculates and plots the density matrix of the Harmonic oscillator. This is used to produce the color plots in figure 7.2.

```
#Importing libraries that may be needed
import numpy as np
import matplotlib.pyplot as pp
import matplotlib.animation as anim
from pylab import *

#Initialization

mx=50               #Matrix elements to be included

wf=np.zeros([mx])   #Initial state vector

wf[25]=1            #26. element nonzero

wf[49]=1            #50. element nonzero

t=1.                #time


#Definitions

def R(t):                       #Define r(t) function
        return np.exp(-t)

def lbn(n,m):                   #Logarithm of binomial coeficient n over m
        return np.sum(np.log(np.arange(n-m+1,n+1))-np.log(np.arange(1,m+1)))

def G(n,m,k,l,r):               #Definition of probagator: (k|(G_t|n)(m|)|l)
        if k<=n and m-l==n-k:
                P=np.abs(r)**2
                return np.exp((lbn(m,l)+lbn(n,k))/2)*(P**l)*((1-P)**(m-l))*(r**(k-l))
        else:
                return 0

#Calculation

rho=np.zeros([mx,mx])       #Density matrix

for n in np.arange(0,mx):
        if(wf[n]!=0):                       #loops through all non-zero n
                for m in np.arange(0,mx):
                        if(wf[m]!=0):       #and all non-zero m
                                for k in np.arange(0,mx):
                                        for l in np.arange(0,mx): #add probagation to all
                                            ellements
```

```
                                    rho[k,l]+=wf[n]*wf[m].conjugate()*G(n,m,k
                                        ,l,R(t))

#Plotting

pcolormesh(rho,cmap='PuBu')          #Make color plot of density matrix
ax=gca()
ax.set_ylim(ax.get_ylim()[::-1])     #Invert y-axis
show()                               #Draw results
```

A.8 Code for calculating $\chi(t)$ and $r(t)$ in the exact solution of the oscillator model

This code calculates $\chi(t)$ and $r(t)$ in the exact solution of the harmonic oscillator model. This is done by diagoanlizing the W matrix as described in section 7.4, and then using the fact that $r(t)$ is the 00 component of the exponentiated matrix, whereas $\chi(t)$ is given by the formula 7.111.

```
#import libraries that may be needed
from pylab import *

#parameters
omega0=2.              #oscillator frequency
omegamax=3.            #maximal environmental frequency
strength=1/(2.*pi)     #strength of interations
T=omega0/log(2)        #temperature
N=3                    #Number of oscillators in environment

t_max=20                                  #time interval
res=300                                   #Plot resolution

#Initialization

omega=linspace(omegamax/N,omegamax,N)  #all environmental frequencies
w=sqrt(strength*omegamax/N)*ones(N)    #all interaction parameters


if T==0:
        b=0
        n=0
else:
        beta=1/T
        b=1/(exp(beta*omega)-1)          #Environmental number expectation
        n=1/(exp(beta*omega0)-1)         #Supposed asymptotic number expectation of S

H=zeros([N+1,N+1])                       #Matrix W
H[0,0]=omega0                            #Oscillator frequency
for i in arange(0,N):
        H[i+1,i+1]=omega[i]              #Frequency    i
        H[i+1,0]=H[0,i+1]=w[i]           #Interaction i

#Calculation

Omega, v = linalg.eig(H)                    #Diagonalizes W
def R(t):                                   #returns vector r at time t
        vt= v[0,0:N+1]*exp(-1j*t*Omega)     #in eigen-basis
        return dot(v,vt)                    #in old basis

def xi(r):                            #Returns xi parameter from vector r
        if T==0:
                return 0
```

```
        else:
                return dot(r[1:N+1],b*conjugate(r[1:N+1]))

t=linspace(0,t_max,res)             #Time interval
r=zeros(res)*1j                     #r parameter
kji=zeros(res)                      #kji parameter

for i in arange(0,res):
        vec=R(t[i])                 #r vector
        r[i]=vec[0]                 #r parameter
        kji[i]=xi(vec)              #kji parameter
```

Bibliography

[1] M.L. Bellac. *Quantum Physics*. Cambridge University Press, 2006.

[2] H.P. Breuer and F. Petruccione. *The Theory of Open Quantum Systems*. Oxford University Press, Incorporated, 2002.

[3] A.O. Caldeira and A.J. Leggett. Path integral approach to quantum brownian motion. *Physica A: Statistical Mechanics and its Applications*, 121(3):587 – 616, 1983.

[4] R. Dümcke and H. Spohn. The proper form of the generator in the weak coupling limit. *Zeitschrift für Physik B Condensed Matter*, 34(4):419–422, 1979.

[5] P.C. Hemmer. *Kvantemekanikk: P.C. Hemmer*. Tapir akademisk forlag, 2005.

[6] L. A. Khalfin. *Sov. Phys. JETP*, 6, 1958.

[7] Jon Magne Leinaas. Non-relativistic quantum mechanics, lecture notes - fys 4110, August 2012.

[8] G. Lindblad. On the generators of quantum dynamical semigroups. *Communications in Mathematical Physics*, 48(2):119–130, 1976.

[9] S. Nakajima. On quantum theory of transport phenomena. *Progress of Theoretical Physics*, 20(6):948–959, 1958.

[10] M.A. Nielsen and I.L. Chuang. *Quantum Computation and Quantum Information*. Cambridge Series on Information and the Natural Sciences. Cambridge University Press, 2000.

[11] John Preskill. Lecture notes for physics 229:quantum information and computation, September 1998.

[12] A. G. Redfield. On the theory of relaxation processes. *IBM Journal of Research and Development*, 1(1):19–31, 1957.

[13] C. Rothe, S. I. Hintschich, and A. P. Monkman. Violation of the exponential-decay law at long times. *Physical review letters.*, 96(16), April 2006.

[14] V. Weisskopf and E. Wigner. Berechnung der natürlichen linienbreite auf grund der diracschen lichttheorie. *Zeitschrift für Physik*, 63(1-2):54–73, 1930.

[15] W. H. Zurek. Pointer basis of quantum apparatus: Into what mixture does the wave packet collapse? *Phys. Rev. D*, 24:1516–1525, Sep 1981.

[16] Robert Zwanzig. Ensemble method in the theory of irreversibility. *The Journal of Chemical Physics*, 33(5):1338–1341, 1960.