Curso 2005/06
CIENCIAS Y TECNOLOGÍAS/1
I.S.B.N.: 84-7756-678-X

INÉS DE VEGA RODRIGO

Relaxation properties in non-Markovian quantum systems

Director
DANIEL ALONSO RAMÍREZ

SERVICIO DE PUBLICACIONES
UNIVERSIDAD DE LA LAGUNA

SOPORTES AUDIOVISUALES E INFORMÁTICOS
Serie Tesis Doctorales

Preface

This thesis contains the work published in several papers during these four years of research. Briefly, the first part of Chapter (5) is based on paper [1], Chapters (8) and (9) contains some of the results of [2] and [3, 4] respectively, and the evolution of quantum mean values in PBG materials developed in Part (IV) is based on [5, 6].

Nevertheless, the present work is not just a juxtaposition of those papers, but we have tried to integrate them into a coherent discourse. In doing so, we have made further contributions. First, we have made an effort to contextualize the results, second, in many cases we have elaborated ideas and arguments beyond the scope of the articles, and third, we have suggested some research possibilities that may be explored in future work.

I. DE VEGA

La Laguna, Islas Canarias

Acknowledgments

Es preciso expresar un profundo agradecimiento a mi director, Dr. Daniel Alonso Ramírez, por haber sido un auténtico maestro durante todos estos años, y por haber creido siempre en mi. Sus enormes cualidades, tanto a nivel personal como profesional, hacen que sea un verdadero privilegio el haber podido trabajar con él. Nunca olvidaré su gran interés y esfuerzo no sólo en que esta tesis saliera adelante, sino también en aportarme una buena formación como investigadora. Gracias, Daniel, por la generosidad y simpatía con la que me has ofrecido tus conocimientos, tu tiempo, tu apoyo y tu entusiasmo.

Part of my first and second year of PHD studies where made in Brussels, where I found an enriching and friendly environment to learn, and to learn how to learn. First of all, I am deeply grateful to Professor Gregoire Nicolis, who gave me his definite support and encouragement to stay in the Centre for Nonlinear Phenomena and Complex systems. Second, but not less important, I have to thank very deeply Professor Pierre Gaspard, for accepting me as his student during that period, for being always available for discussion, and for offering me very interesting remarks and advice.

I have to give very special thanks to Dr. Walter Strunz, for the support he gave me during my whole thesis, and for his hospitality and for all the interesting discussions we had during my visit to Freiburg.

Agradezco muy sinceramente al Dr. Jose María Gómez Llorente su decidido apoyo, gracias al cual ha sido posible obtener la beca FPU que financia esta tesis.

En la quinta planta del edificio de Físicas han transcurrido muchas horas de trabajo, pero también muchos momentos de diversión. Un buen día, entré como novicia en la Sagrada Institución del Café de las Cuatro, (luego felízmente desdoblada en otras tantas), y allí conocí a muchos de los amigos y compañeros que durante todos estos años me han dado descanso, apoyo, y muchas sonrisas: Javi, Santi, Toñi, Eva, José Pascual, Jose Bretón, Rafa, Daniel, Briesta... a todos agradezco profundamente el haberme rescatado, en el momento apropiado, de aquel programa de Fortran o de aquel artículo de difícil digestión.

Quisiera agradecer en especial a José Pascual el apoyo y la amistad mostradas en todo momento, así como a Eva Martín su compañerismo y los buenos ratos que pasamos juntas. También debo dar las gracias en especial a Briesta y a Angel, cuya amistad y alegría me han ayudado a tener un día a día más grato, así como a Javi por su ayuda informática.

A Toñi debo agradecer profundamente su simpatía, su amistad, y la gran generosidad con la que ha dedicado muchas horas de su tiempo en revisar mis artículos y, en el sentido más amplio de la palabra, en ayudarme.

Doy muchas gracias también a Ricardo Florido y a Javier Herrero por su amistad durante todos estos años en los que juntos hemos sufrido las aventuras y desventuras de ser un estudiante de doctorado.

También deseo agradecer su amistad y apoyo a Chano.

Very special thanks go to Massimiliano Esposito for all the interesting discussions we had and for all his helpful remarks about my work, and to Sebastien, for all his help and his kindness. I will always remember their friendship and the enjoyable (and heated) discussions we use to have about politics, philosophy, religion and science.

I'm very grateful to all the people that gave me support and nice moments during my stay in Germany, specially to Andi, Rainer, Wolfgang, Andreas, Jorg and Evers. Special thanks go also to Cord, for showing me always his friendship and his warmness.

A mis buenos amigos de Bruselas, especialmente a Patxi, a Silvia, a Predes, a Sam, a Florence y a Fede, por hacer mi estancia en dicha ciudad algo que recordaré siempre. A Isabelle, mi *angel de la guarda* en Bruselas, por todo su apoyo durante aquel tiempo.

Agradezco profundamente a Irene y a Rebeca el mostrarme siempre, a través de las distintas etapas que han transcurrido a lo largo de estos años, su gran amistad. También agradezco a Marga, a Taida, a May, a Rayco, a Felipe, a Raúl y a Paco los muchos y muy buenos momentos que hemos pasado todos juntos.

¿Qué podría decir de Lola y Julia (Loletta y Jul)? Desde aquel verano tan fresquito de París, pasando por el Hierro, por las Teresas, por el Viana, por el Sin Freno, por la etapa de minimalismo conceptual, por el cinito, por el efecto titi...cuando pienso en los instantes más felices de estos últimos años, siempre estais vosotras. Mas cuando pienso en los momentos más duros, también estais a mi lado, apoyándome. Mil gracias por estar siempre, por hacerme reír, y por quererme.

A Crispi y Carbonilla, por ronronear en los momentos en los que yo ya había perdido la calma.

A Bego, por las comidas ricas, por la compañía, por tantas conversaciones, por ser mi segunda madre.

A mi hermano Miguel, por las divertidas y estimulantes charlas en las que hemos intentado unir (sin conseguirlo del todo) el lenguaje de la ingeniería con el de la física, por disfrutar conmigo en el playuco, por protegerme de los Charlies, por tantos recuerdos felices, y por otros muchos que construiremos juntos. Agradezco a Tanja su gran cariño y apoyo durante todos estos años. Y, lo más importante, mil gracias a los dos por darme las sobrinitas más rubias y simpáticas del Oeste del Rio Pecos, las pequeñas Luci y Clarita.

A mi tía Mercedes, por tener más fe en mí que yo misma, apoyandome en todo momento y haciendome siempre sentir como su *sobrina preferida*.

A los seres queridos que se fueron hace mucho, y aquellos que desaparecieron durante el tiempo en el que escribía esta tesis. En primer lugar, aunque lejana en años, continúa prendida en la memoria la figura de mi abuelito Angel, afable profesor de matemáticas, divertido capataz de aquellos jornaleros que pintabamos la piscina cada verano. Ya más cercano, y siempre presente, está el recuerdo de mi abuelita Rosalía, quien tan orgullosa estuvo siempre de su Inesina, y que veía proyectada en mí la imagen de lo que, con sus capacidades, habría podido hacer con creces, y por sus circunstancias no pudo. También recuerdo a la optimista y cariñosa abuelita Gloria, pendiente siempre de mi carrera, recopilando entusiasmada las noticias del periódico que fueran sobre física. Y mi querido tío Angel, quien fuera mi profe de matemáticas durante algún tiempo, y a quien tanto echaré de menos al final de ésta tesis, dándome un cariñoso *capón* si me equivoco en la lectura.

Debo dar las gracias a toda mi familia, tíos, primos, e hijitos de primos, por hacer siempre de colchón de apoyo y de seguridad, en el que todos sufrimos y somos felices a un solo tiempo.

Finalmente, pero en primer lugar, esta tesis queda dedicada a mis padres, por quererme y apoyarme tanto, y por crecer siempre a mi lado, en cada una de las etapas de mi vida. Desde la nena mofletuda que hacía preguntas, pasando por aquella adolescente que seguía haciendo preguntas, hasta llegar a ser quien soy, alguien que sigue preguntando porqués, pero que tiene algo muy claro: la inmensa suerte de tener unos padres maravillosos.

I.V.R.

Contents

Part I THE REDUCED PROPAGATOR OF A NON-MARKOVIAN QOS

Part II QUANTUM MEAN VALUES

Part III MULTIPLE-TIME CORRELATION FUNCTIONS

Part IV DYNAMICS OF A TWO LEVEL SYSTEM IN A PBG MATERIAL

Part V CONCLUSIONS AND PERSPECTIVES

List of Figures

Acronyms

BEC	Bose-Einstein Condensate
DOS	Density Of States
MTCF	Multiple Time Correlation Functions
PBG	Photonic Band Gap
PC	Photonic Crystal
QOS	Quantum Open System
QRT	Quantum Regression Theorem
QSD	Quantum State Diffusion
SSE	Stochastic Scrödinger Equations
WSC	Wigner-Seitz Cell

Introduction

In general, physical systems (both classical and quantum mechanical) are not found in nature in complete isolation from their environment. For that reason, they may be considered as open systems, and the interaction with the environment may be taken into account in their dynamics.

In order to describe such interaction, one possibility is to integrate the degrees of freedom of the **total system**, composed by the open system and its environment. However, since the number of environmental degrees of freedom is usually very large, to describe all of them may be unpractical (and even impossible). In addition, it would give a large amount of information unnecessary to describe the open system dynamics. In fact, only two quantities may be taken into account in system dynamical equations to describe the effects of the interaction: the environmental vacuum fluctuations, which in some circumstances may be considered as a **noise**, and the autocorrelation function of the vacuum fluctuations, known as the **environmental correlation function**. This function generally decays within so-called correlation time (also *memory time*), which is the time the environment takes to recover from the interaction. Briefly speaking, the noise describes the random effects produced in the system by the large number of environmental degrees of freedom, while the correlation function describes the system dissipation or relaxation to equilibrium, and how this is affected by the environmental memory effects.

A classical system may be described either by its coordinates, or by the probability density of those coordinates. The probability density evolves through a Chapman-Kolmogorov type of equation, which includes a dissipative term that makes it irreversible [7]. The evolution of system variables, particularly position and momentum, may be obtained through a Langevin equation, which in addition to the dissipative term includes a noise term. An average over the different stochastic trajectories obtained through the Langevin equation gives rise to the probability density obtained through the Chapman-Kolmogorov equation. Relaxation properties are particularly important in the comprehension of the appearance of anomalous transport in dynamical systems [8, 9].

In this thesis, we deal particularly with **quantum open systems (QOS)**. Even if the total system is in a pure state, the QOS is a statistical mixture of states which may be described with the so-called **reduced density operator**. Density operators where introduced by Landau in the frame of statistical physics [16], and von-

Neumann [15] for systems far from equilibrium. This operator can be obtained by computing its evolution equation, commonly known as **master equation**, or by performing an average over the different states of a mixture, which are solutions of a **stochastic Scrödinger equation (SSE)**. While a master equation includes dissipative terms, a SSE includes both fluctuation and dissipative terms. Because of them, the Schrödinger equation is no longer unitary and reversible.

A common example of QOS is found in quantum optics, when describing an atom in contact with the radiation field. The interaction produces an exchange of energy between the atom and the field, which in most cases leads to atomic relaxation towards the ground state, and the irreversible loss of its energy into the environmental degrees of freedom.

The atomic relaxation dynamics depends critically on the boundaries and spatial conditions in which the surrounding field is placed. This has been known since the seminal work of Purcell [10], later extended by Kleppner [11], who observed that the relaxation rate of a two level atom placed in a cavity can be enhanced with respect to that of the vacuum, when the radiation wavelength of the emitted photon is comparable to the cavity dimensions, and inhibited when it is far to be comparable. Similar effects may occur within a waveguide. The emission can also be strongly modified when the atom is coupled to a radiation field within a crystal with spatially periodic refraction index. These materials, which were first suggested by Yablonovitch [12] and John [13], are commonly known as **photonic band gap materials (PBG)** or **photonic crystals (PC)**.

How is the atomic dynamics modified by the surrounding spatial and boundary conditions? These dynamics are dependent on the density of field modes around the atomic emission frequency, and it is such density of modes, encoded in the photonic density of states (DOS), that is modified when the field is immersed in a structured environment like a quantum cavity, a waveguide, or a PBG material.

In free space, the photonic density of states is a function that grows with ω^2 and varies in a frequency range which is larger than the atomic spontaneous emission rate. In such conditions, the emitted photon is absorbed instantaneously by the field, which leads to a zero environmental memory time. In that way, the correlation function appearing in the dissipative terms of the atomic dynamical equations is a delta function, and the atom decays exponentially to its ground state as described within the Wigner-Weisskopf theory [14]. This kind of interaction, known as **Markovian** may also occur in a cavity, but again only when the photonic DOS, which has the shape of a Lorentzian, varies smoothly around the atomic emission frequency. In such systems, an enhancement in the spontaneous emission rate occurs for atomic emission frequencies tuned to the Lorentzian maxima or resonance frequency, and a suppression of the emission occurs when the atomic frequency lies far away from the cavity resonance.

In some structured environments, the photonic DOS may present sudden jumps or singular behavior in a frequency range comparable to the spontaneous emission rate. For instance, the periodicity in the refraction index occurring in PC produces the scattering of light outside of the crystal for certain frequencies that are related to the lattice periodicity. Since these modes are absent from the cystal, the photonic DOS is zero in the corresponding frequencies, so that a *gap* is formed. The frequency ranges in which the photonic DOS is non-zero are known as *bands*. In the band edges, the photonic DOS presents a sudden jump from the zero value it has in the gap, to a non-zero value, which gives rise to a group velocity of light that approaches to zero [1]. Hence, when an atom emits a photon in such region, it tends to *freeze* or localize around it, which leads to an eventual reabsortion by the atom. The time in which the environment recovers from the interaction, the memory time, is no longer zero but has a certain finite value which is typical of **non-Markovian** interactions. In non-Markovian interactions the atomic decaying is no longer exponential, and it may even present oscillations due to the exchange of energy between the atomic and photonic degrees

---

[1] The group velocity is given by $v_g = (\partial D(\omega)/\partial\omega)^{-1}$, where $D(\omega)$ is the photonic DOS.

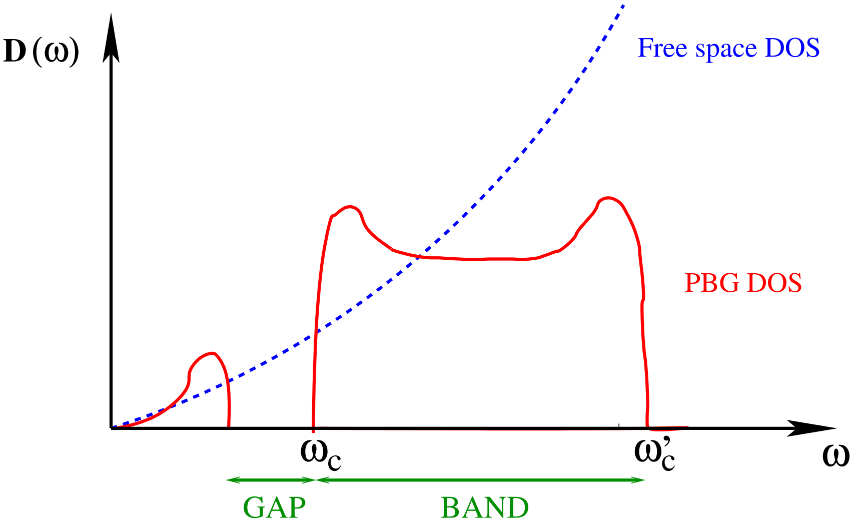

Fig. I.1 Comparison of the photonic DOS of the electromagnetic field in free space, to the photonic DOS typical of a PBG. The latter is characterized by having a gap region where it vanishes $D(\omega) = 0$, and a band, where it is no longer zero and can even present values in which it is larger than the photonic DOS in free space. The singular behavior of the DOS in the band edges can also be observed.

of freedom . This kind of oscillatory (non-Markovian) behavior may also be found in a quantum cavity, when the range of variation of the photonic DOS is comparable to the spontaneous emission rate. Figure (I.1) represents schematically the photonic DOS in a PBG in comparison to that in free space.

In general, master and SSE can be either Markovian or non-Markovian, depending on whether the correlation function appearing in the dissipative term is a delta function or not, and, for SSE, if the noise is a Gaussian white or colored noise. However, although knowledge of the reduced density operator allows calculus of the quantum mean values of system operators, the dynamics of a quantum open system is not only described with such quantities. For instance, in quantum optics some **multiple time correlation functions (MTCFs)** of system observables may be computed to describe quantities such as the atomic emission spectra, or the joint probability of photon detection.

For Markovian interactions, it was discovered by Onsager (especially for the case of fluctuations around equilibrium) [17], and Lax (for the more general case of a system far from equilibrium) [18, 19], that the evolution of two-time correlations can be computed with the master equation for the system reduced density matrix. This result, known as the **Quantum Regression Theorem (QRT)**, can be generalized to N-time correlations, which also obey the same evolution equation as quantum mean values. The atomic emission spectra, which is the Fourier transform of a the two-time correlation of the system coupling operators, is a Lorentzian, as it corresponds to the Fourier transform of an exponential-like decay.

For non-Markovian interactions the emission spectra is no longer just the Fourier transform of the two-time correlation of the coupling operators, but it still depends on such correlation. Nevertheless, the two-time correlations, and in general N-time correlations, can no longer be computed through the QRT. Hence, in non-Markovian interactions the master equation and the reduced density operator are **no longer** the only tool needed to compute all the dynamical quantities of the system. A new theory is needed to derive the dynamical equations of non-Markovian MTCF.

It is the purpose of the present work to study and develop the dynamical equations of a quantum open system linearly coupled to an environment of harmonic oscillators. These include the equations needed to compute quantum mean values, which are mainly the master equation and the SSEs, and the equations that allow the evaluation of MTCFs. The interest in developing such a theory is to be able to describe systems with non-Markovian interactions, like for instance an atom in contact with a structured environment such as the radiation field within a PC.

The work is organized in four parts.

- In Part (I) are two chapters in which the statement of the problem is formulated.

  In Chapter (1), we present the Hamiltonian model studied in this thesis, in which the interaction part represents a linear coupling between system and environment operators. Particularly, it is shown that the interaction Hamiltonian of an atom with the radiation field obeys this linear form, once the rotating wave and dipolar coupling approximations are applied to the general Hamiltonian of a bosonic field in contact with a fermionic field.

  In Chapter (2), we derive the **reduced propagator**, an object that evolves the system wave function conditioned to a certain initial and final state of the environment, and obtain its dynamical equation. This reduced propagator is the essential tool we are going to use during most of this work to derive all the system dynamical equations, for both quantum mean values and multiple-time correlation functions.

- Part (II) is devoted to the study of the quantum mean values of a non-Markovian QOS. It is made up of two chapters:

  In Chapter (4) there is a brief introduction to the different derivations of master and SSE that exist in the literature both for Markovian and non-Markovian interactions, in order to contextualize the particular ones that are used in this work.

  In Chapter (5) we already focus on the study of non-Markovian QOS in two different Sections. In Section (5.1) we study the efficiency of some of the SSEs existing in the literature, an issue that is usually known as the sampling problem. Indeed, certain SSEs give rise to an ensemble of wave vectors with more significant weight in the stochastic sampling of the reduced density operator than other SSEs. For a spin-boson model, we show that the significance of such improvement in the sampling depends on the physical conditions of the total system, particularly on the temperature of the environment. In Section (5.2), we discuss the problem of generating master equations from the evolution equation of the reduced propagator. On the one hand, when the initial state of the environment is considered the vacuum, the reduced propagator gives rise to the usual non-Markovian stochastic Schrödinger equations found in literature, and after an average over the different states of the environment is made, it reproduces the results of the master equation.While the former case has been already treated in literature, our new contribution is to consider a reduced propagator with an initial environmental state different from the vacuum, obtaining a master equation for general initial conditions, and not necessarily for an initially disentangled state for system and environment. The derivation of this master equation implies a generalization of the Novikov theorem, which we also develop in this work.

- Part (III) contains most of the main results of this thesis. A theory of non-Markovian MTCFs is derived from reduced propagators, and also from the Heisenberg equations of motion of system operators.

This part starts by motivating the problem, showing how these MTCFs are very useful in quantum optics to compute quantities such as the emission spectra or photon statistics of an emitting atom. The discussion is divided in two chapters:

In Chapter (8) we show that the non-Markovian MTCF obeys hierarquical structure when no approximations are made. To be more specific, it is found that one-time correlation functions (or quantum mean values), depend on two-time correlations, while two-time correlations depend on three-time correlations. The hierarchy structure is extended to higher order correlations, in such a way that in general, N-time correlations depend on $N + 1$-time correlations. Although this is a formal result which can not be used for computational purposes, it provides a systematic way to derive equations for arbitrary N-time correlations. Those equations become useful for practical purposes once the dependency on higher order correlations is broken by means of some approximation, which is done in the next chapter.

In Chapter (9) we break the hierarchy by assuming a weak coupling approximation, and derive equations for N-time correlations up to second order in the perturbative parameter. This permits us to show that the QRT theorem does not apply for non-Markovian MTCF.

- In Part (IV), some of the equations presented throughout the work are applied to a two level system immersed in the radiation field within a PBG material. The discussion is again divided in two chapters.

  In Chapter (11) an appropriate model for the problem is presented. While the Hamiltonian corresponds to a two level atom dipolarly coupled to a radiation field, and therefore has the same form as the general Hamiltonian presented in Chapter (1), we make some new contributions in the characterization of the environmental correlation function. To this end, we propose a new model of dispersion relation of the field, showing the band-gap periodic structure which is characteristic of the electromagnetic radiation in a PC. Once the correlation function is computed, the corresponding noise can be obtained.

  In Chapter (12) we use the new correlation function and noise to evaluate the quantum mean values of some system operators by integrating the SSE. First, we show that the SSE is equivalent to the master equation which has been traditionally used to study this problem. Second, it is shown that the correlation function we propose gives rise to the same physical effects as the one previously existing in the literature, presenting the advantage that it describes the short time behavior in a more accurate way. Finally, some MTCF are computed, which may be used in future work to derive quantities such as the atomic emission spectra.

- In Part (V) some conclusions and perspectives for future work are drawn.

At the end of the thesis, we include several appendices. These are not essential to follow the work, but complete some of the concepts and the derivations.

We shall make a brief note about the units here used. In Chapter (1) and Appendix (A), where the model for the systems under study is presented, we display the dependencies of all the constants, including $\hbar$. In the rest of the chapters, which are devoted to present and integrate the dynamical equations of those systems, we set for simplicity $\hbar = 1$.

Part I

THE REDUCED PROPAGATOR OF A NON-MARKOVIAN QOS

This part of the work presents two basic concepts, corresponding to each of the chapters: In Chapter (1) the basic model of the systems that are going to be studied is established, namely a quantum open system linearly coupled to an environment of harmonic oscillators through a non-Markovian interaction. In Chapter (2), we present the system reduced propagator, an object that is used in the next parts of the thesis to derive the dynamical equations of quantum mean values and multiple time correlation functions.

1

Non-Markovian quantum open systems

The dynamics of a quantum open system is often described by considering it as a part of a larger **total system** which is isolated from the rest of the world. The Hamiltonian of the total system is denoted by $H_{tot} = H_S + H_B + H_I$, where H_S is the Hamiltonian of the quantum open system (hereafter referred simply as **system**), H_B is the Hamiltonian of its environment, and H_I is the interaction Hamiltonian between the system and environment.

When the environment is large, its evolution time scale may be small in comparison to the relevant time scales of the system. The environment time scale is characterized by the so-called correlation time τ_c, which is the time it takes to recover from the interaction with the system. In the same way, the system time scale is characterized by the time T_A it takes to relax to equilibrium once it is brought into in contact with the environment. There are certain situations in which the separation of time scales is so large that τ_c is practically zero in comparison with T_A. This kind of interaction can be treated with the so-called Markov approximation, and lead to system dynamics that is local in time, i.e. that does not depend on the previous history of the evolution. In other situations the environment correlation time is of the order of T_A, and may significantly influence the dynamics of the open system, making necessary a non-Markovian treatment to describe it. Non-Markovian interactions occur in several contexts, among which we can mention the following examples,

- In **solid state physics** non-Markovian effects are particularly visible in the system dynamics at low temperatures, a fact that will be clarified in Section (1.3.1.2). One of the most generally used models in solid state physics is the one of Caldeira and Legget [20, 22], which describes a harmonic oscillator linearly coupled through its displacement coordinate q to a fluctuating dynamical reservoir or bath, which may represent for instance the phonons of a lattice. In many physical and chemical systems, the generalized coordinate q is associated with an effective potential with two separate minima placed at the same energy. Since only these two states are available, the Hilbert space of the system reduces to a two-dimensional space. This situation, which is described by the so-called spin-boson model, occurs in the motion of light particles in metals, or types of chemical reactions involving electron transfer processes (see [22] and references therein).

- In **quantum optics** non-Markovian effects are present in the emission or absorption of light in the presence of a structured environment. These are electromagnetic fields which are under spatial boundary conditions, like quantum cavities [23, 24, 25, 26], or interacting with a Photonic Band Gap (PBG) material which presents a certain periodicity in the refraction index [27, 28]. An interesting general discussion about the influence of the environmental structure in the atomic dynamics can be found in [29].

- Non-Markovian effects also arise in the dynamics of a **Bose-Einstein condensate** (BEC). In these systems the atoms in the fundamental state are within a trap, and they are coupled by two laser transitions to a final atomic state outside of the trap, so that an atomic "laser" beam is extracted from the BEC. As a particular example of non-Markovian behavior, the dynamics of the occupation number of the BEC exhibit strong oscillations that can be interpreted as a quantum interference effect, and clearly reveal departures from the Golden Rule that predicts exponential decay [30, 31, 32].

Throughout this thesis we mainly study two different sorts of systems: (a) The spin-boson model, valid for the interaction of a two level system with any bosonic reservoir (either phonons or photons) under certain phenomenological conditions. (b) An atom coupled to a radiation field with dipolar interaction. However, the dynamical equations here discussed are valid for a general model of linear system-environment Hamiltonian, and therefore the methodology may be applied to other problems such as the dynamics of Bose-Einstein condensates.

The chapter is organized as follows,

- In Section (1.1) we present the Caldeira and Legget model, as well as the spin-boson model to which it reduces under certain conditions [20, 22, 33, 34]. Within this scheme the interaction Hamiltonian H_I is proportional to SB, where B is an operator belonging to the environment Hilbert space, and $S = q$ is the system coupling operator. The environment coupling operator $B \propto \sum_\lambda g_\lambda \mathcal{F}(a_\lambda, a_\lambda^\dagger)$, where g_λ are the coupling constants of the system with each of the λ harmonic oscillators describing the environment, and $\mathcal{F}(a_\lambda, a_\lambda^\dagger)$ is a particular function of the creation and annihilation operators $a_\lambda^\dagger$ and a_λ.

- The linear interaction Hamiltonian proposed in the Caldeira-Legget model can be generalized as a sum of many system and environment operators, $H_I = \sum_\beta S_\beta B_\beta$. Particulary, it is shown in Section (1.2) how the interaction Hamiltonian between a bosonic field and a fermionic field has this form. An example of this kind of systems is an atom (whose electrons form the fermionic field) dipolarly coupled with the radiation (bosonic) field. In the same way as in the Caldeira and Legget model, the operators B_β are found to be $B_\beta \propto \sum_\lambda g_{\lambda,\beta} \mathcal{F}_\beta(a_\lambda, a_\lambda^\dagger)$. However, in contrast with the former model, in that system the exact dependencies of the coupling constants $g_{\lambda,\beta}$ are known.

  In Section (1.2.1) a new notation is introduced which consists in expressing the interaction Hamiltonian in terms of the so-called Lindblad operators $\{L_\lambda\}$, which represent combinations of the system coupling operators $\{S_\beta\}$. The Hamiltonian of the total system in its Lindblad form, will serve as a general model to develop most of the equations that are used to describe the dynamics of a quantum open system. The argument to use the Lindblad model of Hamiltonian is two-fold: first, as will be explained later, when the interaction is Markovian it gives rise to a master equation that preserves positivity for the reduced density operator of the system, the so-called Lindblad equation, and second, it is one of the most often used Hamiltonians when studying quantum open systems.

- Some aspects concerning the so called **correlation function**, $\alpha(t)$, and the **spectral density**, $J(\omega)$, are shown in Section (1.3), specially those that determine whether the interaction is Markovian or non-Markovian.

The environmental correlation function is a very important quantity to describe the system dynamics, first because it appears in its dynamical equations, and second because it determines the environmental relaxation time τ_c. It is proportional to a sum of the square of the coupling constants of the system, $\alpha(t) \propto \sum_\lambda g_\lambda^2 \mathcal{P}(t, \omega_\lambda)$, with $\mathcal{P}(t, \omega_\lambda)$ a certain function that will be specified later.

In the continuum, this sum is transformed into an integral where the kernel is the so-called spectral density, $J(\omega)$, in such a way that $\alpha(t) = \int d\omega J(\omega)\mathcal{P}(t, \omega)$. Since $\mathcal{P}(t, \omega)$ has the same form for any system, the spectral density basically contains the same information as the correlation function, and just in the same way it characterizes the environment and its interaction with the system.

In Section (1.3.1) we describe the two different methods to derive the correlation function.

The first is called *microscopic* since it relies on the knowledge of the form of the coupling constants. As an illustration, we use the g_λ's that characterize the interaction of a two level atom with the vacuum radiation field, to derive a Markovian correlation function. Within that interaction, the spectral density $J(\omega)$ is found to be a smoothly varying function of frequency in comparison with the atomic spontaneous emission decay rate Γ, so that it can be considered approximately a constant. More complicated microscopic calculus of the correlation function correspond to interactions of an atom with structured environments. Those systems are typically non-Markovian, since the spectral density changes on a frequency scale comparable to the spontaneous emission rate and can not be considered a constant. Some examples are treated in next chapters.

When the exact form of the couplings is not known, as happens in the Caldeira and Legget model, a second method is needed which consists in deriving the spectral density $J(\omega)$ according to several *phenomenological* arguments. As an example, we discuss the $J(\omega)$ that is used in this thesis to describe the spin-boson model.

It is important to note that none of the derivations presented in this chapter are original. For that reason, most of them are not shown in their complete version, and therefore the reader interested in further details should go to the original references. The main goal is to give the ideas and the proper references to derive the Hamiltonian of the physical systems that are studied in this work, namely the spin-boson model and an atom in contact with a radiation field. The main results of the thesis concern the development and study of the dynamical equations describing non-Markovian quantum open systems, and therefore these models are only useful as examples in which such equations are applied. An exception to this is the two level atom immersed in a PBG material, where we make some contributions to the model. Since, in addition, the PBG system presents interesting new physics, it deserves special treatment and will be explained in detail in Part (IV).

1.1 CALDEIRA-LEGGET MODEL

We shall consider in this section the general Hamiltonian of a system with one or few degrees of freedom coupled to a bath of harmonic oscillators as described in [20, 22, 33, 34]. The Hamiltonian of the total system is the following,

$$H_{tot} = H_S + H_B + H_I \tag{1.1}$$

where the Hamiltonian of the system with generalized coordinate q is

$$H_S = \frac{P^2}{2M} + V(q), \tag{1.2}$$

with P and M the momentum and mass of the particle respectively, and the Hamiltonian of the bath of harmonic oscillators is

$$H_B = \sum_\lambda \left(\frac{1}{2} \frac{p_\lambda^2}{m_\lambda} + \frac{1}{2} m_\lambda \omega_\lambda^2 x_\lambda^2 \right). \tag{1.3}$$

Here, the p_λ and x_λ are the momentum and position coordinates of the λ harmonic oscillator. The interaction of the system with each mode of the reservoir is proportional to the inverse volume of the reservoir, so that for a spatially large environment this coupling is small. Therefore, it is a good approximation for macroscopic environments to consider that the system-reservoir coupling is a linear function of the bath coordinates, so that the interaction Hamiltonian has the form

$$H_I = -\sum_\lambda F_\lambda(q) x_\lambda + \Delta V(q). \tag{1.4}$$

In the former Hamiltonian, a counterterm has been added to renormalize the potential $V(q)$. Indeed, in presence of the interaction, the minima of the potential for a given q is displaced a certain quantity, in such a way that the effective potential in (1.2) is $V_{eff}(q) = V(q) - \Delta' V(q)$. Renormalization consists in making $\Delta V(q) = \Delta' V(q)$, so that the minima of the potential is replaced to its initial value. For the special case of a separable interaction [22],

$$F_\lambda(q) = C_\lambda F(q), \tag{1.5}$$

and the simplest case in which $F(q) = q$, the total Hamiltonian is written as

$$H_{tot} = \frac{P^2}{2M} + V(q) + \frac{1}{2} \sum_\lambda \left[\frac{p_\lambda^2}{m_\lambda} + m_\lambda \omega_\lambda^2 \left(x_\lambda - \frac{C_\lambda}{m_\lambda \omega_\lambda^2} \right)^2 \right], \tag{1.6}$$

where the renormalization factor is identified as

$$\Delta V(q) = \frac{C_\lambda^2}{m_\lambda \omega_\lambda^2} q^2. \tag{1.7}$$

Replacing (1.5) in (1.4), the interaction term of the Hamiltonian (1.6), without the renormalization term, has the general form

$$H_I = BS \tag{1.8}$$

with $B = -\sum_\lambda C_\lambda x_\lambda$ and $S = F(q) = q$. The Hamiltonian (1.6) has been widely used to describe dissipation in open quantum systems and is often referred in literature as the Caldeira-Legget model [22, 34].

From the Caldeira and Legget it is possible to derive the Hamiltonian of a two level atom in contact with a harmonic environment, namely a spin-boson model. There are some systems where the potential function $V(q)$ appearing in (1.6) has the form of a double well with two separated minima. When certain conditions in the parameters are fulfilled by the two wells and the barrier between existing between them, the Hilbert space of the system can be reduced to a two state space, and the problem simplifies considerably. These systems are often referred as *truncated* two state systems [34]. Let us now explain briefly the conditions for obtaining a truncated two state system. Consider $\hbar\omega_2$ and $\hbar\omega_1$ as the energy separation between ground and excited level of left and right well respectively, and V_0 the height of the potential barrier. If ω_0 is of the order of magnitude of ω_2 and ω_1, the first condition to be fulfilled is

$$V_0 >> \hbar\omega_0, \tag{1.9}$$

so that when both wells are put in contact with each other through the potential barrier $\hbar\omega_2$ and $\hbar\omega_1$ remain approximately constant. The second condition assures that the system is effectively restricted to the two level system conformed by the ground levels of both wells. For that reason, no thermal excitations to the upper levels of both wells should be allowed,

$$\kappa_B T \ll \hbar\omega_0, \tag{1.10}$$

while the energy difference between the two levels, $\hbar\omega_{12} = |\omega_2 - \omega_1|\hbar$ is considered much smaller with respect to ω_0 and arbitrary with respect to the thermal energy $\kappa_B T$. In addition, the two states can be weakly coupled through a transfer o tunneling matrix element Δ_0, giving rise to oscillations in the population of the left and right well that are responsible for quantum interference effects.

Apart from truncated two level systems, there exist *intrinsical* two state systems, for instance a nucleus of spin $1/2$, or a photon with two polarization states.

When any two level system (both intrinsecal or truncated) is in contact with an environment which can be modeled as a bath of bosons (for instance a phononic bath or an electromagnetic field), the global system is considered a spin-boson model, and has the following Hamiltonian

$$H_{tot} = H_{SB} = \frac{1}{2}\hbar\omega_{12}\sigma_z - \frac{1}{2}\hbar\Delta_0\sigma_x + H_B + BS, \tag{1.11}$$

where the interaction term has the form (1.8) with $B = \sum_\lambda C_\lambda x_\lambda$ as the environment coupling operator, and the system coupling operator S depends on the particular model considered. Expressing the former Hamiltonian in terms of creation and annihilation operators,

$$H_{SB} = \frac{1}{2}\hbar\omega_{12}\sigma_z - \frac{1}{2}\hbar\Delta_0\sigma_x + \sum_{\lambda=1}^{N}\hbar\omega_\lambda a_\lambda^\dagger a_\lambda + \sum_{\lambda=1}^{N}\hbar g_\lambda(a_\lambda + a_\lambda^\dagger)S, \tag{1.12}$$

since $x_\lambda = \sqrt{\frac{\hbar}{2m_\lambda\omega_\lambda}}(a_\lambda + a_\lambda^\dagger)$, and $p_\lambda = -i\sqrt{\frac{\hbar m_\lambda\omega_\lambda}{2}}(a_\lambda - a_\lambda^\dagger)$. From now on, we will use the constant $g_\lambda = \sqrt{\frac{1}{2\hbar m_\lambda\omega_\lambda}}C_\lambda$ as the coupling parameter.

1.2 BOSONIC-FERMIONIC FIELD INTERACTION HAMILTONIAN

In the former section we have shown how the Hamiltonian of a quantum open system in contact with an environment of harmonic oscillators can be modeled with a simple form (1.1), by choosing a linear interaction of the form (1.8). A particular H_S and H_I was given for the case of a two-level system coupled with the environment through a single Hermitian operator S. In this section we show how the coupling Hamiltonian H_I can be generalized by considering it as a sum of many linear couplings between a set of bath operators, $\{B_\alpha\}$, and system operators, $\{S_\alpha\}$ [35],

$$H_I = \sum_{\beta=1}^{M} B_\beta S_\beta, \tag{1.13}$$

which we assume Hermitian. Despite this assumption, the Hamiltonian (1.13) is quite general, as shown in Section (1.2.2). We derive the interaction Hamiltonian between a bosonic field and a fermionic field, showing how it is reduced to the form (1.13). From now on, we will often refer the bosonic field as a radiation field, and the fermionic field as an electron wave field. With this particular choice the atom-photon interaction is described, since an atom interacts with the radiation field through its electrons. Particularly, the interaction of the electron wave field of a single electron, with the radiation field is equivalent to the problem of a single electron atom interacting with an electromagnetic field.

Let us follow the derivation presented in [21]. In order to give a quantized theory of the interaction, the electron is quantized in a similar way as the electromagnetic field. A general wave function for the electron field $\Psi(\mathbf{r})$ may be expanded in terms of a complete set of wave functions ϕ_j obeying the Schrödinger equation

$$H_{el}\phi_j(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\bigtriangledown^2 + eV(\mathbf{r})\right)\phi_j(\mathbf{r}) = E_j\phi_j(\mathbf{r}), \tag{1.14}$$

where $V(\mathbf{r})$ is the Coulomb potential, and the interaction between electrons has been neglected. Thus, we can expand $\Psi(\mathbf{r})$ in such a set as

$$\Psi(\mathbf{r}) = \sum_j b_j\phi_j(\mathbf{r}). \tag{1.15}$$

By analogy with the quantization of the light field the expansion coefficients b_j will become operators in the quantized electron field, and $\Psi(\mathbf{r})$ becomes a field operator. The basis functions obey the orthonormality relations

$$\int \phi_i^*(\mathbf{r})\phi_j(\mathbf{r}) = \delta_{ij}. \tag{1.16}$$

The Hamiltonian describing the interaction between the electromagnetic field and an electron field, discarding the spin of the electron, is

$$\tilde{H}_{tot} = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}(\mathbf{r}))^2 + eV(\mathbf{r}) + H_B, \tag{1.17}$$

where e and m are the electronic charge and mass respectively, $\mathbf{p}$ is the momentum of the electron, and $\mathbf{A}$ is the vector potential of the electromagnetic field. When the electron wave field is quantized, the last Hamiltonian becomes

$$H_{tot} = H_{el} + H_{I1} + H_{I2} = \int d^3r\Psi^\dagger(\mathbf{r})\tilde{H}_{tot}\Psi(\mathbf{r}), \tag{1.18}$$

where

$$\begin{aligned} H_{el} &= \int d^3r\Psi^\dagger(\mathbf{r})\left[\frac{-\hbar^2}{2m}\bigtriangledown^2 + eV(\mathbf{r})\right]\Psi(\mathbf{r}), \\ H_{I1} &= \int d^3r\Psi^\dagger(\mathbf{r})\left[-\frac{e}{m}\mathbf{A}(\mathbf{r})\cdot\mathbf{p}\right]\Psi(\mathbf{r}), \\ H_{I2} &= \int d^3r\Psi^\dagger(\mathbf{r})\left[-\frac{e}{m}\mathbf{A}^2(\mathbf{r})\right]\Psi(\mathbf{r}). \end{aligned} \tag{1.19}$$

Since $H_{el}\phi_j(\mathbf{r}) = E_j\phi_j(\mathbf{r})$, with E_j the electronic energy corresponding to the state ϕ_j, we have

$$H_{el} = \sum_{jk} b_j^\dagger b_k E_k \int d^3r\phi_j^*(\mathbf{r})\phi_k(\mathbf{r}) = \sum_j E_j b_j^\dagger b_j, \tag{1.20}$$

because following (1.16) the basis functions are orthogonal, and

$$H_{I1} = \sum_{jk} b_j^\dagger b_k \int d^3r \phi_j^*(\mathbf{r}) \left[-\frac{e}{m} \mathbf{A}(\mathbf{r}) \cdot \mathbf{p} \right] \phi_k(\mathbf{r}), \tag{1.21}$$

with

$$\mathbf{A}(\mathbf{r}) = \sum_\lambda \sqrt{\frac{\hbar}{2\omega_\lambda \epsilon_0}} \left[a_\lambda \mathbf{A}_\lambda(\mathbf{r}) + a_\lambda^\dagger \mathbf{A}_\lambda^*(\mathbf{r}) \right]. \tag{1.22}$$

The term H_{I2} is discarded, being negligible for processes of one photon. The functions $\mathbf{A}_\lambda(\mathbf{r}) \equiv \mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r})$ appearing in (1.22) are the mode functions of the electromagnetic field, which may in general be any complete set of basis functions spanning the region under consideration. In free space, one might consider the basis functions as simple plane waves

$$\mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r}) = \sqrt{\frac{1}{v}} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\mathbf{e}}_{\mathbf{k}\sigma}, \tag{1.23}$$

where $\hat{\mathbf{e}}_{\mathbf{k}\sigma}$ is the unit vector in the direction of the polarization state σ for a given wave vector $\mathbf{k}$, and v is the quantization volume. In Part (IV) will be studied how this basis functions should be chosen as Bloch modes for the case of a radiation field immersed in a photonic band gap material. The reason is that within such materials the translation symmetry characteristic of free space is broken, and the radiation modes present periodicity in the wave vector $\mathbf{k}$. In any case, the expansion (1.23) is valid even in that case, provided that we are restricted to a single cell of the reciprocal lattice, i.e. the first Brillouin zone. At this point, in order to proceed with the calculus, we put the Hamiltonian (1.21) in terms of the so-called coupling strenghts $g_{\lambda,j,k}$,

$$g_{\lambda,j,k} = -\frac{e}{m} \sqrt{\frac{1}{2\hbar\omega_\lambda \epsilon_0}} \int d^3r \phi_j^*(\mathbf{r}) \left[\mathbf{A}_{\mathbf{k},\sigma}(\mathbf{r}) \cdot \mathbf{p} \right] \phi_k(\mathbf{r}), \tag{1.24}$$

so that

$$H_{I1} = \hbar \sum_{\lambda,j,k} b_j^\dagger b_k \left(g_{\lambda,j,k} a_\lambda + g_{\lambda,j,k}^* a_\lambda^\dagger \right). \tag{1.25}$$

The coupling strengths can be further simplified by considering that the mode functions in the position of the electron $\mathbf{r}$, given by (1.23), can be replaced to first approximation by its value in the position of the atomic nucleus $\mathbf{r}_0$

$$\mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r}) = \sqrt{\frac{1}{v}} e^{i\mathbf{k}\cdot\mathbf{r}_0} \left(1 + i\mathbf{k}\cdot\delta\mathbf{r} - \frac{(\mathbf{k}\cdot\delta\mathbf{r})^2}{2} \right) \hat{\mathbf{e}}_{\mathbf{k}\sigma} \propto \sqrt{\frac{1}{v}} e^{i\mathbf{k}\cdot\mathbf{r}_0} \hat{\mathbf{e}}_{\mathbf{k}\sigma}. \tag{1.26}$$

This approximation, also known as the electric dipole approximation, is justified in the optical region, since in that range the wavelength of the photon is much greater than the linear dimension of the atom $\hat{\lambda}_{photon} = \frac{1}{|\mathbf{k}|} \gg \mathbf{r}_{atom}$, since $\hat{\lambda}_{photon} \sim 10^3 \dot{A}$, and $\mathbf{r}_{atom} \sim 1\dot{A}$. Additionally, the coupling strenghts can be further simplified by considering that $\mathbf{p} = \frac{im}{\hbar}[H_{el}, \mathbf{r}]$, and also the fact that $\{\phi_j\}$ are eigenfunctions of H_{el} with eigenvalues ω_j. With this consideration and the dipole approximation, we have

$$g_{\lambda,j,k} = -i\sqrt{\frac{1}{2\hbar\omega_\lambda \epsilon_0}} \omega_{jk} \mathbf{A}_{\mathbf{k},\sigma}(\mathbf{r}_0) \cdot \mathbf{d}_{jk}, \tag{1.27}$$

where $\omega_{jk} = \frac{E_j - E_k}{\hbar} = \omega_j - \omega_k$, and

$$\mathbf{d}_{jk} = e \int d^3 r \phi_j^*(\mathbf{r}) \mathbf{r} \phi_{\mathbf{k}}(\mathbf{r}), \tag{1.28}$$

is the dipolar moment. As shown in Appendix (A), a different coupling constant $g_{\lambda,j,k}$ is obtained by using a gauge dependent Hamiltonian. If we now choose the phase of $\mathbf{A}_{\mathbf{k},\sigma}(\mathbf{r}_0)$ in (1.27) so that $g_{\lambda,j,k}$ is real, the total Hamiltonian is

$$H_{tot} = \sum_j E_j b_j^\dagger b_j + \sum_\lambda \hbar\omega_\lambda a_\lambda^\dagger a_\lambda + \hbar \sum_{\lambda,j,k} g_{\lambda,j,k} b_j^\dagger b_k \left(a_\lambda + a_\lambda^\dagger \right), \tag{1.29}$$

where the first and second terms corresponds to the electron and photon field respectively, and the last term H_I corresponds to the interaction between them. Notice that such interaction is already of the form (1.13), i.e a sum in $\beta \equiv \{j,k\}$ of Hermitian system operators $S_\beta \equiv b_j^\dagger b_k$ and Hermitian environmental operators $B_\beta \equiv g_{\lambda,j,k}(a_\lambda + a_\lambda^\dagger)$. For a single electron in contact with the photonic field, $g_{\lambda,2,1} = g_{\lambda,1,2}$, and therefore we have

$$H_I = \hbar \sum_\lambda g_{\lambda,1,2} \left(a_\lambda + a_\lambda^\dagger \right) \left[b_1^\dagger b_2 + b_2^\dagger b_1 \right], \tag{1.30}$$

which is again of the form (1.13). In the last expression, the coupling constant are given by

$$g_{\lambda 1,2} = -i \sqrt{\frac{1}{2\hbar\epsilon_0\omega_\lambda}} \omega_{12} \mathbf{A}_\lambda(\mathbf{r}_0) \cdot \mathbf{d}_{12}. \tag{1.31}$$

1.2.1 Lindblad form for the interaction Hamiltonian

It is often convenient to put the general H_I given by (1.13), in terms of the so-called Lindblad operators $\{L_\gamma\}$, with $\gamma = 1, \cdots, P$, that are operators belonging to the system Hilbert space, but not necessarily Hermitian. The Lindbland form Hamiltonian is interesting, first because it permits generation of an evolution equation for the system reduced propagator $\rho_S = Tr_B(\rho_{tot})$ that in the Markov limit reduces to the Lindblad master equation [36] which has been shown to preserve positivity [37, 38], and second, because it is quite a general model, since many system-environment interaction Hamiltonians reduce to this form once the necessary hypothesis are made. For instance, in the case we have described above of a photon field in contact with an electron field, the necessary approximation for arriving to the Lindbland form is, apart from the dipolar approximation, the so-called rotating wave approximation. Thus, let us consider two cases in the Hamiltonian (1.29),

- When $j < k$, the electron operator $b_j^\dagger b_k$ gives rise to a decay from the upper level E_k to the lower E_j, and the emission of a photon. As a consequence, in order to conserve the energy, it is necessary that this term is accompained with a creation operator for the photonic field, $a_\lambda^\dagger$, where the photon frequency is $\omega_\lambda = \omega_{jk}$. The term $b_j^\dagger b_k a_\lambda$ is discarded, since it would correspond to the highly non-energy-conserving process of annihilating two photons simultaneously in both electron and photon field.

- When $j > k$, $b_j^\dagger b_k$ corresponds to a electronic excitation that should be accompained with the annihilation of a photon in the field represented by the operator a_λ. The terms $b_j^\dagger b_k a_\lambda^\dagger$ corresponds to the simultaneous creation of a photon in both fields, which may be neglected in comparison to one-photon processes.

When expressing the Hamiltonian (1.29) in the interaction picture, it is found that the terms that are not discarded, also known as resonant terms, rotate with frequencies $\omega_\lambda - \omega_{jk}$, whereas the neglected terms rotate much faster with frequencies of order $\omega_\lambda + \omega_{jk} = 2\omega_\lambda$. Within the rotating wave approximation, the interaction Hamiltonian appearing in (1.29) is expressed in Lindblad form as

$$H_I = \hbar \sum_\lambda \sum_\gamma g_{\lambda,\gamma} \left(a_\lambda L_\gamma^\dagger + a_\lambda^\dagger L_\gamma \right), \tag{1.32}$$

with the Lindblad operators defined as

$$L_\gamma = b_j^\dagger b_k, \tag{1.33}$$

where $\gamma \equiv j, k$ with the condition $j > k$. For a single electron in contact with the photonic field we have

$$H_I = \hbar \sum_\lambda g_\lambda \left[\sigma_{21} a_\lambda + \sigma_{12} a_\lambda^\dagger \right], \tag{1.34}$$

for (1.30), where we have considered that $g_\lambda \equiv g_{\lambda,2,1} = g_{\lambda,1,2}$, and the electron operators expressed in pseudo-spin operators, where $\sigma_{21} \equiv \sigma^+ = b_2^\dagger b_1$ is the rising operator, and $\sigma_{12} \equiv \sigma^- = b_1^\dagger b_2$ is the lowering operator.

1.2.2 Relation between different linear interaction Hamiltonians

In this section we show how the Hamiltonian (1.13) is in fact the most general form of linear interaction Hamiltonian. The derivation is based in a result appearing in [37]. Indeed, any interaction Hamiltonian in terms of non-Hermitian operators, H_I', can be expressed in terms of Hermitian operators assuming the form H_I of (1.13). Since the Lindblad Hamiltonian, here referred as $H_I'^{Lin}$, is a specific case of H_I', the derivation is also useful to relate the Hamiltonian (1.32) with (1.13). Suppose that we have

$$H_I' = \sum_{\beta=1}^{N} S_\beta' B_\beta', \tag{1.35}$$

where contrary to (1.13) the system and environmental operators (S_β' and B_β') are not Hermitian. The Hamiltonian in the general form (1.35) (and also in its Lindblad form (1.38) with the choice (1.39) for the operators), can be expressed as a sum of Hermitian operators by simply setting,

$$\begin{aligned} \tilde{S}_\beta &= \frac{1}{2}\left(S_\beta' + S_\beta'^\dagger \right) \; \tilde{\tilde{S}}_\beta = \frac{i}{2}\left(S_\beta' - S_\beta'^\dagger \right) \\ \tilde{B}_\beta &= \frac{1}{2}\left(B_\beta' + B_\beta'^\dagger \right) \; \tilde{\tilde{B}}_\beta = -\frac{i}{2}\left(B_\beta' - B_\beta'^\dagger \right), \end{aligned} \tag{1.36}$$

so that the interaction Hamiltonian becomes written inthe form (1.13),

$$H_I = \sum_{\beta=1}^{N} \left(\tilde{S}_\beta \tilde{B}_\beta + \tilde{\tilde{S}}_\beta \tilde{\tilde{B}}_\beta \right) = \sum_{\beta=1}^{2N} S_\beta B_\beta \tag{1.37}$$

with

$$\begin{aligned} S_\beta &= \tilde{S}_\beta & \forall\, \beta = 1, N \\ S_\beta &= \tilde{\tilde{S}}_{\beta-N} & \forall\, \beta = N+1, 2N, \end{aligned} \tag{1.38}$$

and

$$\begin{aligned} B_\beta &= \tilde{B}_\beta \qquad && \forall\, \beta = 1, N \\ B_\beta &= \tilde{\tilde{B}}_{\beta - N} \qquad && \forall\, \beta = N+1, 2N. \end{aligned} \tag{1.39}$$

The Lindblad form of (1.35) corresponds to the case in which (a) $N = 2p$, so that

$$H'_I = S'_1 B'_1 + S'_2 B'_2 + \cdots + S'_{2p-1} B'_{2p-1} + S'_{2p} B'_{2p}, \tag{1.40}$$

and (b) the coupling operators are related by couples in such a way that

$$\begin{aligned} S'_{p+1} &= S'^{\dagger}_1 ; \cdots S'_{2p} = S'^{\dagger}_{p-1} \\ B'^{\dagger}_{p+1} &= B'_1 ; \cdots B'^{\dagger}_{2p} = B'_{p-1}. \end{aligned} \tag{1.41}$$

Relabeling the former elements, we have

$$H'^{Lin}_I = L_1 E^\dagger_1 + L^\dagger_1 E_1 + \cdots + L_p E^\dagger_p + L^\dagger_p E_p = \sum_{\gamma=1}^{p} \left(L_\gamma E^\dagger_\gamma + L^\dagger_\gamma E_\gamma \right), \tag{1.42}$$

where

$$\begin{aligned} S'_1 &= L_1,\, S'_2 = L_2,\ \cdots S'_p = L_p, \\ S'_{p+1} &= L^\dagger_1,\, S'_{p+2} = L^\dagger_2,\, \cdots S'_{2p} = L^\dagger_p \\ B'_1 &= E_1,\, B'_2 = E_2,\ \cdots B'_p = E_p, \\ B'_{p+1} &= E^\dagger_1,\, B'_{p+2} = E^\dagger_2,\, \cdots B'_{2p} = E^\dagger_p. \end{aligned} \tag{1.43}$$

Note that in (1.32) the environmental operators are $E_\gamma = \hbar \sum_\lambda g_{\lambda,\gamma} a_\lambda$.

To transform the Lindbland Hamiltonian into the form (1.37), it is necessary to take into account in (1.36) that $\tilde{S}_1 = \frac{1}{2}(S'_1 + S'^{\dagger}_1) = \frac{1}{2}(S'_{p+1} + S'^{\dagger}_{p+1}) = \tilde{S}_{p+1}$. Therefore,

$$H^{Lin}_I = 2 \sum_{\beta=1}^{p} \left(\tilde{S}_\beta \tilde{B}_\beta + \tilde{\tilde{S}}_\beta \tilde{\tilde{B}}_\beta \right) = \sum_{\beta=1}^{N} S_\beta B_\beta, \tag{1.44}$$

with

$$\begin{aligned} S_\beta &= 2\tilde{S}_\beta \qquad && \forall\, \beta = 1, p \\ S_\beta &= 2\tilde{\tilde{S}}_{\beta - p} \qquad && \forall\, \beta = p+1, 2p, \end{aligned} \tag{1.45}$$

and

$$\begin{aligned} B_\beta &= \tilde{B}_\beta \qquad && \forall\, \beta = 1, p \\ B_\beta &= \tilde{\tilde{B}}_{\beta - p} \qquad && \forall\, \beta = p+1, 2p. \end{aligned} \tag{1.46}$$

Let us for instance derive the form (1.44) (or (1.13)) for a the case of a single Lindblad operator. In that case, since $p = 1$ then $M = 2$. Then

$$S_1 = L + L^\dagger \, ; \, S_2 = i(L - L^\dagger), \tag{1.47}$$

and

$$B_1 = \frac{1}{2}\sum_\lambda g_\lambda(a_\lambda + a_\lambda^\dagger)\,;\; B_2 = \frac{i}{2}\sum_\lambda g_\lambda(a_\lambda - a_\lambda^\dagger). \tag{1.48}$$

Notice that B_1 and B_2 are proportional to a sum over x_λ and p_λ respectively, and that all the $\{B_\beta\}$ and the $\{S_\beta\}$, with $\beta = 1, 2$, are effectively Hermitian. It can be checked with the replacement of (1.47) and (1.48) in (1.13), that we arrive to the Lindblad Hamiltonian

$$H_{tot} = H_S + H_B + \sum_\lambda g_\lambda(L^\dagger a_\lambda + La_\lambda^\dagger). \tag{1.49}$$

The relations (1.47) and (1.48) will be useful in Chapter (II) when the Stochastic Schrödinger equation derived by Pierre and Nagaoka in [35] for an interaction in the form (1.13) is compared to that derived in [39, 40, 41] for an H_I of the form (1.49). In addition, the last Hamiltonian will be used as an essential piece for starting the derivation of most of the dynamical equations presented in this work. Indeed, the equations derived for (1.49) are very appropriate for describing linear coupling, since the results are easily generalized by considering a sum over the set of Lindblad operators, L_γ.

1.3 CHARACTERIZATION OF THE RESERVOIR: RELEVANCE OF NON-MARKOVIAN INTERACTIONS

We discuss in this section the different forms of the spectral function $J(\omega)$, as well as its relation with the correlation function $\alpha(t)$ which characterizes the system-environment interaction. Additionally, some ways to derive $J(\omega)$ are presented. At this stage of the exposition we will remain qualitative, and only give the reader some ideas to understand the two different kind of interactions, Markovian and non-Markovian, existing between system and environment. Further details of the derivations, as well as computation of $J(\omega)$ (or alternatively $\alpha(t)$) for particular systems are given in the next chapters.

An important quantity to characterize the influence of the environment on the system dynamics is the so-called spectral function $J(\omega)$, defined as

$$J(\omega) = \hbar\pi\sum_\lambda g_\lambda^2\delta(\omega - \omega_\lambda) \tag{1.50}$$

where g_λ are the coupling strengths defined in the former sections. In the limit of large number of oscillators $g_\lambda \to g(\omega)$, and the (1.50) may be considered in the continuum as,

$$J(\omega) = g^2(\omega)D(\omega), \tag{1.51}$$

where $D(\omega)$ is the photonic density of states (DOS). The function $J(\omega)$ defines the environmental correlation function $\alpha(t)$. For instance, for a Hamiltonian (1.49) with $L = L^\dagger$ and a thermal reservoir in equilibrium, $\alpha(t)$ is defined as

$$\alpha(t) = \int_0^\infty d\omega J(\omega)\left[\coth\left(\frac{\omega\beta}{2}\right)\cos(\omega t) - i\sin(\omega t)\right], \tag{1.52}$$

where $\beta = (\kappa_B T)^{-1}$, with κ_B the Boltzmann constant and T the environmental temperature. For $T = 0$ the correlation function becomes simply a Fourier transform of the function $J(\omega)$

$$\alpha(t) = \int_0^\infty d\omega J(\omega)e^{i\omega t}. \tag{1.53}$$

The behavior of the open system depends quite strongly on the shape of $\alpha(t)$ and therefore of $J(\omega)$. The reason is that the environmental correlation function appears in all the system dynamical equations, both in those that describe the dynamics of its expectation values and in those describing the dynamics of its fluctuations. It acts as the kernel of integral terms over the past history of the system evolution.

Thus, the correlation function is responsible for the dependency of the system's evolution over its past history. As previously noted, when the decaying time of the correlation function, namely the environmental correlation time, τ_c, is comparable to the evolution time of the system, T_A, the interaction is considered non-Markovian. The interaction is Markovian when the correlation time is practically zero compared to T_A, so that $\alpha(t-\tau)=\Gamma\delta(t-\tau)$, with $\Gamma=1/T_A$ the system relaxation rate. In Markovian interactions the memory of the system evolution over its history disappears.

The correlation time τ_c is determined by the shape of the spectral density. Let us see this more carefully by considering the following possibilities for $J(\omega)$,

- $J(\omega)$ is composed by the sum of a *finite* number of harmonic oscillators. Hence, the correlation function might decay within a time τ_c, but revival is observed after the so-called recurrence time τ_R. The oscillators define a spectrum and τ_R is roughly determined by the inverse of ΔE_{min}, the minimum separation between energies. In that way, the less harmonic oscillators there are, the larger is ΔE_{min} and the smaller is τ_R. In some situations, τ_R can be smaller than the time in which the system energy is dissipated, so that a revival is observed in its dynamics. This means that the system may dissipate to a certain state, but may be re-excited by the environment after a certain time τ_R. It can also be the case that τ_R is even smaller than τ_c, in which case such correlation time can not even be properly defined. In summary, a $J(\omega)$ composed of a small number of oscillators usually gives rise to a highly non-Markovian interaction.

- $J(\omega)$ composed by an *infinite* sum of harmonic oscillators. The corresponding frequency spectrum is sufficiently dense as to produce an infinite recurrence time. Dissipation is therefore observed (except for very special situations like an atom with rotating frequency placed in the gap of a photonic band gap material), and there are no revival effects in the system dynamics. Nevertheless, the interaction is Markovian only when, in addition, the spectral function is smoothly varying function of ω particularly within the region nearby the characteristic frequencies of the open system. Otherwise, when $J(\omega)$ changes abruptly along that region, it gives rise to a correlation function that might decay within a time of the order of the atomic decaying time. This situation may be produced by a $D(\omega)$ which exhibits a sudden jump or some weaker kind of singular non-analytic behavior. This occurs, for example, in a waveguide close to its fundamental frequency, or nearby the band edge of a PBG. In the last case, the photonic DOS of the radiation field presents two kind of regions: a gap where $D(\omega)$ vanishes, and a band where the density of states is non-zero, but present a rapid variation with frequency near the gap, as does $J(\omega)$.

If the correlation time τ_c cannot be defined, the interaction should not be treated by using a perturbative approximation. It will become clear in the next chapter that the perturbative parameter and the correlation time are related with each other. Thus, the larger the environmental relaxation time is, the smaller has to be the coupling between system and environment in order to perform a perturbative expansion [1]. Obviously, when τ_c is not even defined (for instance because $\tau_R<\tau_c$), it means that the environmental relaxation time should be taken to be infinite, and therefore the coupling between system and environment may be zero in order to justify the use of a perturbative expansion. This situation will only be studied for special

---

[1] To be more precise, when τ_c is large, it is necessary either to arrive to high orders the perturbative expansion, or to have a small perturbation parameter.

choices of coupling operators L which gives rise to exact solutions and therefore do not need the use of any approximation, particularly the perturbative approximation.

1.3.1 Derivations of the spectral function

There are two different possibilities to determine the spectral function $J(\omega)$, depending on the particular model.

As noted above, when the environment is a continuum reservoir of harmonic oscillators and the quantum open system can be described by a single extended coordinate q, the spectral function can be determined *phenomenologically*, particularly from the knowledge of the coefficients of the classical equation of motion [22, 34].

For more general environments that shall not necessarily be reservoirs (i.e. that shall not be infinite), and for more general systems than those described by a single coordinate q, a *microscopical* knowledge of the interaction is needed to derive $J(\omega)$. Particularly, to perform the sum (1.50), it is necessary to know the form of the coupling constants g_λ.

In the next sections we present the microscopic derivation of the correlation function for Markovian interactions, and a phenomenological derivation of the model of $J(\omega)$ we are going to use in this thesis when studying the spin-boson system.

1.3.1.1 Microscopic Here we present a microscopic derivation of the correlation function for an atom interacting with an electromagnetic field in the simplest case in which the interaction is Markovian. More complicated microscopic derivations of $J(\omega)$, or equivalently of the environmental correlation function are presented in the next chapters for non-Markovian interactions. For instance, in Part (IV) the correlation function which describes the atomic interaction with an electromagnetic field immersed in a photonic crystal is obtained.

In general, a microscopic derivation is possible for atoms interacting with electromagnetic fields since the coupling constants are given by (1.24) for a dipolar coupling between levels $|j\rangle$ and $|k\rangle$. The coupling constants corresponding to the interaction of a two level atom with the electromagnetic field are expressed in (1.31) as,

$$\begin{aligned} g_{\lambda 1,2} &= -i\sqrt{\frac{1}{2\hbar\epsilon_0\omega_\lambda}}\omega_{12}\mathbf{A}_\lambda(\mathbf{r}_0)\cdot\mathbf{d}_{12} = \\ &\quad -i\sqrt{\frac{1}{2v\hbar\epsilon_0\omega_\lambda}}\omega_{12}e^{-i\mathbf{k}\cdot\mathbf{r}_0}d_{12}\hat{\mathbf{e}}_\lambda\cdot\hat{\mathbf{d}}_{12}, \end{aligned} \tag{1.54}$$

where we have inserted $\mathbf{A}_\lambda(\mathbf{r}_0) = \sqrt{\frac{1}{v}}e^{-i\mathbf{k}\cdot\mathbf{r}_0}\hat{\mathbf{e}}_\lambda$ to go from the first to the second line. Let us now take equation (1.53) in its discrete version,

$$\alpha(t) = \sum_\lambda |g_\lambda|^2 e^{-i\omega_\lambda t}. \tag{1.55}$$

The sum in λ is in fact a sum over the two polarization modes, denoted by σ and the electromagnetic wave vector $\mathbf{k}$. In the continuum limit, we then have

$$\sum_\lambda \equiv \sum_\sigma \sum_{\mathbf{k}} \rightarrow 2\frac{v}{(2\pi)^3}\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta \int_0^\infty dk k^2, \tag{1.56}$$

where the factor 2 in the last expression comes from the sum in σ. From (1.54), we have

$$g_\lambda^* g_\lambda = \frac{1}{2\hbar\omega_\lambda \epsilon_0 \upsilon}\omega_{12}^2 d_{12}^2 \cos^2\theta, \tag{1.57}$$

where $|\hat{\mathbf{e}}_{k,\sigma}\cdot\hat{\mathbf{d}}_{12}|^2 = \cos^2\theta$, and θ is the angle between the atomic dipole moment $\hat{\mathbf{d}}_{12}$ and the electric field polarization vector $\hat{\mathbf{e}}_{k\sigma}$. Replacing (1.57) together with (1.56) in (1.55), we have

$$\alpha(t) = 2\frac{\upsilon}{(2\pi)^3}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dk \frac{k^2}{2\upsilon\hbar\omega(k)\epsilon_0}\omega_{12}^2 d_{12}^2 \cos^2\theta e^{-i\omega(k)t}, \tag{1.58}$$

where we have also assumed that the dispersion relation is such that $\omega(\mathbf{k}) = \omega(k)$. Considering the dispersion relation of an electromagnetic field in the vacuum, we have $k = \omega/c$, and we can easily transform the k integral into a frequency integral,

$$\alpha(t) = \frac{2}{3}\int_0^{\infty} d\omega \frac{\upsilon\omega^2}{(2\pi)^2 c^3}\frac{\omega_{12}^2 d_{12}^2}{4\upsilon\hbar\omega\epsilon_0} e^{-i\omega t} \tag{1.59}$$

where we have already solved the angular integrals. From the last expression, we can already identify the photonic density of states as

$$D(\omega) = \frac{\upsilon\omega^2}{(2\pi)^2 c^3}, \tag{1.60}$$

and the function $g^2(\omega)$

$$g^2(\omega) = \frac{\omega_{12}^2 d_{12}^2}{6\upsilon\hbar\omega\epsilon_0}, \tag{1.61}$$

so that following (1.51), the spectral function is

$$J(\omega) = \frac{\upsilon\omega^2}{(2\pi)^2 c^3}\frac{\omega_{12}^2 d_{12}^2}{6\upsilon\hbar\omega\epsilon_0}. \tag{1.62}$$

In terms of $J(\omega)$, and from (1.51), the correlation function (1.59) is expressed as

$$\alpha(t) = \int_0^{\infty} d\omega J(\omega) e^{-i\omega t} \approx J(\omega_{12}) 2\pi\delta(t), \tag{1.63}$$

where $\int_0^\infty d\omega e^{-i\omega t} = 2\pi\delta(t)$. The last expression contains the crucial approximation which characterizes Markovian interactions. This consists in considering $J(\omega) = D(\omega)g^2(\omega)$ approximately constant nearby the atomic rotating frequency ω_{12}, and equal to $J(\omega_{12})$. Notice that this is only justified for interactions such that the variation of the spectral function $J(\omega)$ is smoothly varying function nearby the atomic rotating frequency. For instance, in a PBG material this situation only occurs when ω_{12} is placed in the middle of a band which is sufficiently broad as to make the band border effects negligible.

Since the correlation function appears as a kernel in the integral terms of the system dynamics that are responsible of the dissipation, it determines its relaxation time T_A. Particularly, the correlation function fixes the system decay rate Γ as

$$\Gamma = \int_0^{\infty} d\tau \alpha(\tau), \tag{1.64}$$

where $T_A = \Gamma^{-1}$. For a Markovian system with (1.63), the decay constant is

$$\Gamma = 2\pi J(\omega_{12}) = \frac{d_{12}^2 \omega_{12}^3}{6\pi\hbar\epsilon_0 c^3}. \tag{1.65}$$

The fact that $\alpha(t)$ depends on $F(\omega) = g^2(\omega)D(\omega)$ explains why the spontaneous decaying of atoms is not fully characterized by intrinsical atomic properties, but by quantities such as the photonic DOS of the surrounding radiation field, and the coupling strengths with each of the harmonic oscillators that form the environment.

The importance of the medium in the atomic emission was first pointed out by Purcell in 1946 [10], who predicted that the spontaneous emission rate of a cavity containing atoms becomes enhanced in the case of atom-cavity resonance. Atoms in the cavity may therefore radiate spontaneously faster than in free space. This can be explained more clearly by considering that the photonic density of states of the radiation field in a cavity with resonance placed in the atomic rotating frequency is [43]

$$D^{cav}(\omega) = \frac{1}{\pi} \frac{\omega/2Q}{(\omega_{12} - \omega) + (\omega/2Q)^2}, \tag{1.66}$$

where Q is the so-called quality factor of the cavity on which the enhancement depends. Now suppose that the atomic rotating frequency is placed nearby the lowest cavity mode, so that $\omega_{12} \propto \pi c/L$, where L is the length of the side of the cavity. In that region, the former photonic DOS simplifies as

$$D^{cav}(\omega_{12}) = 2Q/\pi\omega_{12} \propto \frac{2LQ}{\pi^2 c}, \tag{1.67}$$

so that we have,

$$\Gamma^{cav} = 2\pi g^2(\omega_{12}) D^{cav}(\omega_{12}) = \frac{2d_{12}^2 Q}{3\hbar\epsilon_0 \upsilon}, \tag{1.68}$$

where we have also inserted (1.61) evaluated at ω_{12}. Comparing the former decaying rate with that of the vacuum, given by (1.65), we have,

$$\Gamma^{cav} = \Gamma Q \left(\frac{2\pi c^3}{\varphi \omega_{12}^3} \right). \tag{1.69}$$

Considering the lowest cavity mode, $\omega_{12} = \frac{\pi c}{L}$, the former expression is simplified as

$$\Gamma^{cav} = \Gamma Q \frac{2}{\pi^2}, \tag{1.70}$$

where we have also considered $\upsilon = L^3$. Considering that the factor $\frac{2}{\pi^2}$ is of order one, the last relation shows that the spontaneous emission rate of an atom in a quantum cavity is enhanced by a factor Q with respect to that of the vacuum. In the same way, if atomic transitions are far from any cavity resonance, the spontaneous emission process will be inhibited. The same kind of inhibition of spontaneous emission occurs if atoms are located in a waveguide and their transition frequency is below the fundamental frequency of the waveguide [11, 44]. In the same way, this picture shows that the spontaneous emission rate can be enhanced in a photonic band gap material, since there are frequency ranges where $D(\omega)$ can be larger than in free space. Additionally, within the gap $D(\omega) = 0$, which in turn means that $\Gamma = 0$. In other words, single photon spontaneous emission is completely inhibited. This implies that the vacuum fluctuations or zero-point fluctuations are absent for frequencies inside a gap, and thus, within the forbidden frequency band the PBG materials are emptier than even the vacuum.

This rough picture of spontaneous emission is equivalent to the one that follows from the Fermi Golden rule [45, 46]. The spontaneous emission rate $\mathcal{W}_{fi} \equiv \Gamma$ for an atom initially in the excited state $|i\rangle$ to a final state $|f\rangle$ after the emission of a single photon of wavevector $\mathbf{k}$ (and therefore $\lambda = \mathbf{k}, \sigma$) is

$$\mathcal{W}_{fi} = \frac{2\pi}{\hbar} |\langle H_{i,\mathbf{k}} \rangle|^2 D(\omega_{12}), \tag{1.71}$$

where $H_{i,\mathbf{k}} = g_{\mathbf{k}}(\mathbf{r}_0)(a_{\mathbf{k}} L^\dagger + L a^\dagger_{\mathbf{k}})$ and $g_\lambda(\mathbf{r}_0) = 2 g_{\mathbf{k}}(\mathbf{r}_0)$. A comparison of (1.65) together with (1.51) leads to the conclusion that $g^2(\omega_{12}) = \frac{2\pi}{\hbar} |\langle H_{i,\mathbf{k}} \rangle|^2$.

Before ending with this section, we should stress again that the above picture is very approximate for non-Markovian processes, since it assumes that $D(\omega)$ and $F(\omega)$ are smooth varying functions in the region nearby the atomic resonant frequency compared with Γ. For instance, in the above example of a quantum cavity, when the cavity decay rate is much less than the atomic spontaneous emission rate there will be an oscillatory exchange of the energy between the atomic and the photonic degrees of freedom before the spontaneously emitted photon leaks out of the cavity. This is no longer the typical Markovian exponential decaying with rate Γ given by the Fermi Golden Rule.

In the next section we give an example of phenomenological derivation of the spectral function, as described by Legget and co-workers in [34].

1.3.1.2 Phenomenological In order to obtain a spectral function for the Caldeira-Legget Hamiltonian (1.6), it is necessary to make some phenomenological approximations, since the exact form of the coupling coefficients C_λ is in principle not known. To do that, it is possible to extract some parameters form the classical evolution equation for the generalized coordinate of the system, q, namely the generalized Langevin equation [22]

$$M\ddot{q}(t) + V'(q) + M \int_0^t dt' \gamma(t - t') \dot{q}(t') = \hat{\zeta}(t), \tag{1.72}$$

where $V'(q) = \frac{\partial V}{\partial q}$, and M is the mass of the system. The function $\hat{\zeta}(t) = \zeta(t) - M\gamma(t) q(0)$, where $q(0)$ is the initial value of the generalized coordinate and

$$\zeta(t) = \sum_\lambda C_\lambda \left(x_\lambda^{(0)} + \frac{p_\lambda^{(0)}}{m_\lambda \omega_\lambda} \sin(\omega_\lambda t) \right), \tag{1.73}$$

with $x_\lambda^{(0)}$ and $p_\lambda^{(0)}$ the initial values of the environmental coordinates. Taking the average of the initial values $x_\lambda^{(0)}$ and $p_\lambda^{(0)}$ with respect to the canonical classical equilibrium density of the unperturbed reservoir, $\rho_B^{(0)} = Z^{-1} \exp(-\beta H_B)$

$$\rho_B^{(0)} = Z^{-1} e^{-\beta \sum_\lambda \left(\frac{p_\lambda^{(0)^2}}{2m_\lambda} + \frac{m_\lambda \omega_\lambda^2}{2} x_\lambda^{(0)^2} \right)}, \tag{1.74}$$

where Z is the partition function, the function $\zeta(t)$ becomes a fluctuating force with Gaussian statistical properties,

$$\begin{aligned} \langle \zeta(t) \rangle_{\rho_R^{(0)}} &= 0 \\ \langle \zeta(t) \zeta(t') \rangle_{\rho_R^{(0)}} &= M \kappa_B T \gamma(t - t'). \end{aligned} \tag{1.75}$$

Given its relation with $\zeta(t)$, then the quantity $\hat{\zeta}(t)$ is also a Gaussian noise with the same properties. The second equality of (1.75) is an example of the classical fluctuation-dissipation theorem [16], which expresses the relation between the fluctuating quantities $\hat{\zeta}(t)$ appearing in (1.72), and the dissipative function or memory friction kernel $\gamma(t)$, which is responsible of the lost of energy from system to environment. Such function is defined as

$$\gamma(t-t') = \Theta(t-t')\frac{1}{M}\sum_{\lambda}\frac{C_{\lambda}^{2}}{m_{\lambda}\omega_{\lambda}^{2}}\cos\left(\omega_{\lambda}(t-t')\right), \tag{1.76}$$

where $\Theta(t-t')$ is the step function introduced to ensure causality. Taking into account that $C_{\lambda} = \sqrt{2\hbar\omega_{\lambda}m_{\lambda}}g_{\lambda}$, and inserting the definition (1.50) of the spectral function in the last expression, we get

$$\gamma(t-t') = \Theta(t-t')\frac{2}{\pi M}\int d\omega\frac{J(\omega)}{\omega}\cos\left(\omega(t-t')\right). \tag{1.77}$$

The microscopic properties encoded in the function $J(\omega)$ can now be expressed in terms of the phenomenological damping kernel $\gamma(t)$ by only applying the inverse Fourier transform in the last expression,

$$J(\omega) = M\omega\int_{0}^{\infty}dt\gamma(t)\cos\left(\omega t\right). \tag{1.78}$$

The Markovian limit corresponds to a flat reservoir, which gives rise to a Fourier transform of the friction kernel, $\hat{\gamma}(\omega) = \int_0^\infty dt\gamma(t)\cos\left(\omega t\right) = \gamma$, so that

$$J(\omega) = \omega M\hat{\gamma}(\omega) = \omega\eta, \tag{1.79}$$

where $\eta = M\gamma$ is a dissipative coefficient with the dimensions of viscosity. The Markovian case corresponds to what is referred in literature as *ohmic* damping, in which $J(\omega) \propto \omega$. However, it is often the case that we find non-Markovian reservoirs in which on one hand the spectrum is not flat, and on the other hand, the memory friction kernel is not known, so that $J(\omega)$ cannot be fixed with the use of (1.78). In those cases, it is always possible to assume that the spectral function behaves in the short frequency limit as ω^s,

$$J(\omega) = \eta_s\omega^s\omega_c^{1-s}e^{-\omega/\omega_c}, \tag{1.80}$$

where $0 < s < 1$ in the *sub-ohmic* case, and $s > 1$ in the *super-ohmic* [34]. The constant η_s has the dimensions of viscosity and is equal to $M\gamma_s$, where γ_s is the dissipative coefficient for the particular choice of s which can be obtained from (1.76) as $\gamma_s = \int_0^\infty dt\gamma_s(t)$. The exponential factor appearing in the last expression has been added to provide a smooth cut-off for the spectral density, which is modulated by the frequency ω_c. Although the cutoff frequency shall be conveniently chosen in accordance with other scales and parameters of the problem, it turns out that the dependency of all the physical results on ω_c cancel out for a vast range of the parameter space. Whether we have *ohmic*, *sub-ohmic* or a *super-ohmic* spectral function depends on the type of reservoir, and determines quite strongly the evolution behavior of the coupled system. For instance, the case of ohmic friction is important for charged intersticials in metals. A phonon bath in d spatial dimensions corresponds to the case $s = d$ or $s = d + 2$ depending on the symmetry properties of the field. Non integral values of s may be relevant for fractal environments. Further examples of different systems in interaction with environments that falls in these three categories, as well as the description of their dynamics are found in [20, 22, 34]. For the spin-boson model studied in this thesis, we will consider a superohmic reservoir with $s = 3$,

$$J(\omega) = \frac{\omega^3}{\omega_c^2}e^{-\omega/\omega_c}. \tag{1.81}$$

Let us now discuss the properties of the model (1.81). The temperature plays an important role to determine the relevance of non-Markovian effects within the system dynamics. As displayed in Fig (1.1), decreasing the temperature (i.e. increasing β) gives rise to an increase of the maximum of the real part of the correlation function (1.50), through the coefficient $\coth(\frac{w_\lambda}{2kT})$. The real part reflects then the magnitude of the environmental thermal fluctuations. In the limit of zero temperature such coefficient is one, and the magnitude of the real part of the correlation is equivalent to the imaginary part, both corresponding to purely quantum fluctuations. As mentioned before, the correlation function enters in all the system dynamical equations, and its real part is responsible of the dissipation which leads the system to an equilibrium state. In that way, lower temperatures give rise to less dissipation, which means that the system takes a larger time T_A to relax. Since the effects of a finite correlation time τ_c operates at very short time scales, it is obvious that they will be more visible when the system decays slowly. In other words, a slow decaying permits to see some structure in the relaxation, which is due to non-Markovian effects occurring at the short time scale τ_c. On the contrary, a rapid decaying erases these non-Markovian effects.

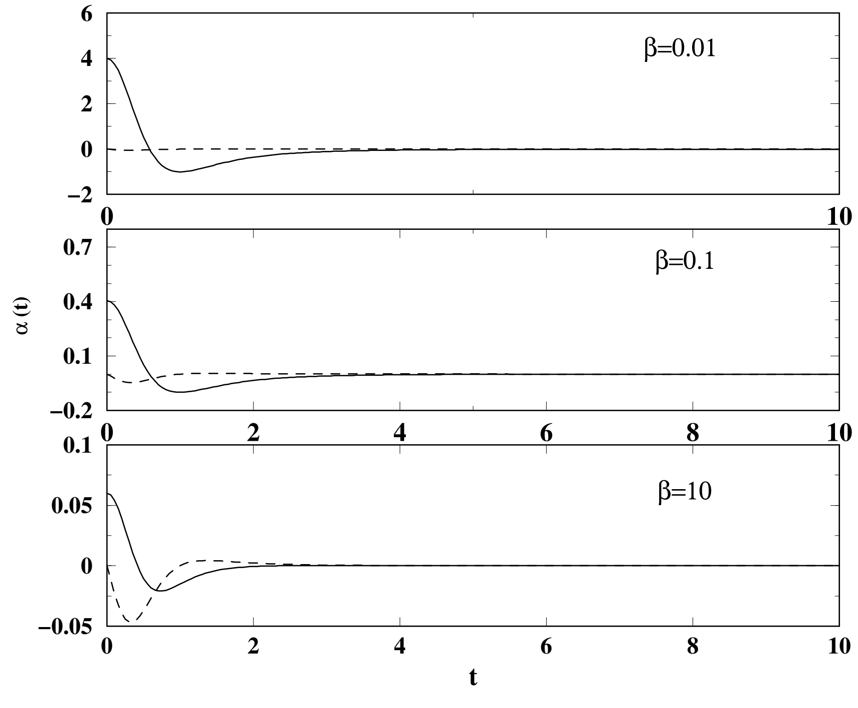

Fig. 1.1 Correlation function displayed for different temperatures. The imaginary part is displayed in dashed line, while the real part is in continuous line. The correlation time is the same for high temperatures (small β) than for low temperatures (large β). Nevertheless, as the temperature becomes smaller the magnitude of the correlation function (specially of its real part, which is responsible of the dissipation) becomes smaller, so that the system takes a longer time T_A to relax to equilibrium. Because of that, although the correlation time τ_c remains the same, non-Markovian effects are more present at low temperatures.

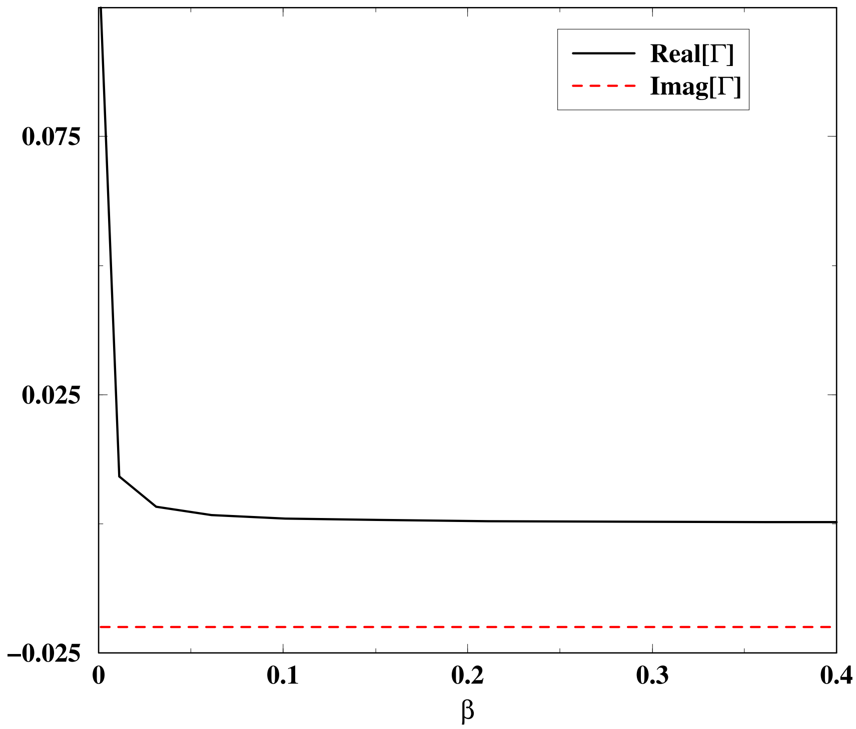

Fig. 1.2 Spontaneous decay rate Γ of the system displayed for different temperatures. Non-Markovian effects are visible in the system dynamics when the variation of $J(\omega)$ nearby the resonance frequency is comparable to the spontaneous decay rate of the system Γ. For a high temperature the coefficient Γ is so high that it would be necessary a very rapid variation of $J(\omega)$ to observe non-Markovian effects in the dynamics.

2

The reduced propagator of a QOS

We present in this chapter the **reduced propagator**, an object that evolves the system wave function conditioned to a certain initial and final state of the environment. The reduced propagator is an essential tool to derive the dynamical equations which describe a QOS interacting with its environment. First, when the initial state of the environment is taken the vacuum, the reduced propagator gives rise to the usual non-Markovian stochastic Schrödinger equations found in literature. Also, after an average over the different initial and final states of the environment, it reproduces the master equation. Second, when the initial state of the environment is not the vacuum, the reduced propagator gives rise to a master equation for general initial conditions (and not necessarily a decorrelated state between system and environment), and to the evaluation of system fluctuations.

2.1 INTRODUCTION

The reduced propagator permits us to derive all the dynamical equations for a non-Markovian quantum open system. This includes not only the evolution of its expectation values, but also of its fluctuations. The reduced propagator, denoted as $G(z_i^* z_{i+1}|t_i t_{i+1})$, is the matrix element of the total evolution operator in the Bargmann coherent basis of the environment [47], $\{|z_i\rangle = |z_{i,1} \cdots, z_{i,\lambda} \cdots\rangle\}$. Hence, it lives in the Hilbert space of the system. Furthermore, it represents transitions between the environmental state z_{i+1} to z_i. In that way, when applied to the system wave function, it $propagates$ the system state from an initial time t_{i+1} to a final time t_i, $conditioned$ that the environmental state is initially in $|z_{i+1}\rangle$ and finally in $|z_i\rangle$.

The evolution of **expectation values** (also quantum mean values) have been widely described both for Markovian and non-Markovian interactions. Two equivalent schemes are currently used. The first consists in evolving the reduced density matrix of the system, defined as a trace over the environmental degrees of freedom of the total system density matrix, through some master equation [22, 38, 50, 51, 52, 53]. In the Markovian case, the reduced density matrix has been shown to preserve positivity when the master equation is expressed in the Lindblad form [36]. The second scheme has been developed more recently, and consists in the so-called *stochastic Schrödinger equation* (SSE) that evolves state vectors in such a way that an average over an ensemble of solutions equals the reduced density matrix. In the Markov case, the stochastic term of SSE can have the form of discontinuous jumps randomly interrupting the evolution, or a diffusive term acting continuously every time step of the evolution. This last type of SSE has been extended to treat non-Markovian interactions. The reduced propagators derived in this thesis can be used to derive a non-Markovian diffusive SSE, provided that the initial and final environmental states, z_{i+1} and z_i are chosen randomly according to their distribution [41, 3, 4].

Apart from expectation values, **fluctuations** (also multiple-time correlation functions, MTCF) of system observables are found in the dynamical description of different phenomena, such as in the atomic emission spectra or the statistics of emitted photons. In the Markov case, the knowledge of the evolution of the system reduced density matrix is sufficient to derive both quantum mean values and MTCF. This result, known as Quantum Regression Theorem (QRT) [50, 51, 53], has been also derived by using SSE [56, 57, 58, 59]. Nevertheless, as we show in this thesis this is no longer the case for non-Markovian interactions, which have to be computed with some new equations. Although there do exist some numerical methods to evaluate non-Markovian MTCF, for instance the one proposed by Breuer in [60, 61], before our work there had not yet been derived the evolution equation for those quantities. Reduced propagators becomes a basic tool to compute such evolution equations [2, 3, 4].
This chapter is organized as follows:

- Section (2.2) shows how the reduced propagator $G(z_i^* z_{i+1}|t_i t_{i+1})$ can be used to obtain:
  - The evolution of the reduced density matrix $\rho_s(t)$. In order to do this, it is necessary to perform an average over the environment initial and final states (z_{i+1} and z_i respectively).

    This can be done $numerically$, by considering that since there is a very large number of these states, they can be chosen randomly according to the environment state distribution. The reduced propagator becomes a *stochastic propagator*, and its evolution equation a SSE.

    Alternatively, it is possible to perform the sum *analytically*, so that a master equation for $\rho_s(t)$ can be obtained. The object $G(z_i^* 0|t_i 0)$ has been already introduced in literature by Strunz in [41] as a stochastic propagator. Since it corresponds to the particular case in which the initial environmental state is the vacuum, $z_{i+1} = 0$, it will be here referred to as *vacuum propagator*. The vacuum propagator corresponds to the SSE derived in [40, 41, 54], and has been already used in literature to derive analytically master equations (see for instance [6, 54, 55]). However, all these equations keep the restriction that the initial environmental state has to be the vacuum[1]. The reduced propagator $G(z_i^* z_{i+1}|t_i t_{i+1})$ permits the derivation of more general master equations corresponding to other environments (like for instance a thermal reservoir), or even to initially correlated states for the environment and system. The derivation of some of these master equations is made in Part (II).
  - The evolution of non-Markovian MTCF, by performing *numerically* an average over different trajectories. However, the advantage of reduced propagators is that this average can also be done *analytically* which gives rise to a set of evolution equations of the MTCF within the weak coupling limit. These equations clearly show that only a set of particular multiple-time correlation functions satisfy the Quantum Regression Theorem (QRT), whereas in general MTCF do not. It is important to stress that the computation of MTCF can only be done with propagators where the initial environmental state, $|z_{i+1}\rangle \neq |0\rangle$, which makes vacuum propagators unsuitable. The complete derivation of the theory of MTCF is discussed in Part (III).

---

[1] In [40] a SSE is derived for thermal environments, but it is not derived from reduced propagators. This equation is presented in Part (II), and compared to the one derived in [35] also for thermal environments.

The reduced propagator is, then, a very useful tool to derive any aspect of the dynamic of a QOS, provided that its evolution equation is obtained. This is done in the next sections:

- In Section (2.3) an **open equation** is derived: Since the system and its environment are entangled, the dynamics of the first is conditioned to particular environmental states. In addition, such entanglement gives rise to an evolution equation for the system reduced propagator that is not closed. To be more specific, it does not depend only on the reduced propagator that is being evolved but on a family of these corresponding to different initial and final environmental states. Due to this dependency over other propagators, this equation is referred in this thesis as open equation.
- In Section (2.4) a **closed equation** is derived: For non-Markovian interactions the dependency on other trajectories of propagators only disappear in special systems which have an exact solution. This systems are those with diagonal coupling operator in the free Hamiltonian basis, i.e. $L \propto H_S$. In general systems, some approximations have to be made. We show some of these approximations that are needed to obtain a closed equation for the reduced propagator, namely the expansion, the weak coupling and the near-Markov approximations. It also becomes clear in this section that the entanglement between trajectories occurs during the correlation time τ_c, and therefore disappears in the Markovian limit.

Some comments about the numerical and analytical way to obtain an average over reduced propagators are made in Section (2.5).

From now on and throughout the rest of the thesis (except where indicated), we take $\hbar = 1$.

2.2 REDUCED PROPAGATOR: A TOOL TO COMPUTE THE DYNAMICS OF A QOS

As noted in the first chapter, a frequently used Hamiltonian model in the study of the dynamics of $\mathcal{S}$ with Hamiltonian H_S, in interaction with H_I is

$$\begin{aligned} H_{tot} &= H_S + H_B + H_I \\ &= H_S + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda + \sum_\lambda g_\lambda \left(a_\lambda^\dagger L + L^\dagger a_\lambda \right), \end{aligned} \tag{2.1}$$

where the operator L acts on the Hilbert space of the system and $a_\lambda, a_\lambda^\dagger$ are the annihilation and creation operators on the environment Hilbert space. The $g_\lambda' s$ are the coupling constants that can be taken as real numbers, and the $\omega_\lambda' s$ are the frequecies of the harmonic oscillators that constitute the environment [20]. Instead of a single system coupling operator L in H_I we could consider a set of them, but such generalization is straightforward and does not affect the conclusions we shall derive in this thesis. The wave function corresponding to the total Hamiltonian (2.1), evolves from its initial value $\mid \Psi_0\rangle$ as,

$$\mid \Psi_t\rangle = \mathcal{U}_I \mid \Psi_0\rangle \tag{2.2}$$

where $\mathcal{U}_I(t,0)$ is the evolution operator in interaction picture,

$$\mathcal{U}_I(t,0) = e^{iH_B t} e^{-iH_{tot} t}. \tag{2.3}$$

We can represent the state (2.2) in an environmental basis, which is here chosen as the Bargmann coherent state basis (see Appendix (B) for a explanation of the coherent and Bargmann basis) [47, 48]. Thus, the total system state can be expressed as [41, 43],

$$\mid \Psi_t\rangle = \int d\mu(z_i) G(z_i^* 0|t0)|\psi_0\rangle|z_i\rangle. \tag{2.4}$$

In the last expression we have used the Gaussian measure

$$d\mu(z_i) = \prod_{\lambda} \frac{d^2 z_{i,\lambda}}{\pi} e^{-|z_{i,\lambda}|^2}, \tag{2.5}$$

and we have used the notation $\mid z_i\rangle =\mid z_{i,1}\rangle \mid z_{i,2}\rangle ... \mid z_{i,\lambda}\rangle ...$ for the state of the environment, given by a tensorial product of the states of all the λ environmental oscillators. The basis states for each oscillator are, in terms of the number states basis $\mid z_{i,\lambda}\rangle = \exp(z_{i,\lambda} a^{\dagger}_{i,\lambda}) \mid 0\rangle$. The function

$$G(z_i^* 0|t0) = \langle z_i \mid \mathcal{U}_I(t,0) \mid 0\rangle, \tag{2.6}$$

with $\mathcal{U}_I(t,0)$ given by (2.3), is the vacuum reduced propagator, that was interpreted by Strunz in [41] as a "stochastic propagator". Vacuum reduced propagators gives rise to a displacement of the wave function from its initial value $\mid \psi_0\rangle$, to the value $\mid \psi_t(z_i^*)\rangle$ at time t, provided that the environment oscillators have evolved from the vacuum state $\mid 0\rangle$ to the state $\mid z_i\rangle$. Mathematically, this is expressed as $G(z_i^* 0|t0) \mid \psi_0\rangle =\mid \psi_t(z_i^*)\rangle$. For other situations in which the environment is not initially in the vacuum and the evolution time does not start at zero, a more general propagator is needed [3]. Such propagator is obtained by representing the system evolution operator $\mathcal{U}_I(t_i, t_{i+1})$, with $t_i > t_{i+1}$ in the Bargmann coherent state basis [47],

$$G(z_i^* z_{i+1}|t_i t_{i+1}) = \langle z_i \mid \mathcal{U}_I(t_i, t_{i+1}) \mid z_{i+1}\rangle. \tag{2.7}$$

Here $\mid z_{i+1}\rangle$ represents the initial state of the environment at time t_{i+1}, and $\mid z_i\rangle$ its final state at time t_i. The interaction picture evolution operator $\mathcal{U}_I(t_i, t_{i+1})$ is defined as

$$\mathcal{U}_I(t_i, t_{i+1}) = e^{iH_B t_i} e^{-iH_{tot}(t_i - t_{i+1})} e^{-iH_B t_{i+1}}. \tag{2.8}$$

Therefore, the *reduced propagator* $G(z_i^* z_{i+1}|t_i t_{i+1}) = \langle z_i|\mathcal{U}_I(t_i, t_{i+1})|z_{i+1}\rangle$ acts on the system Hilbert space, giving the evolution of system state vectors from t_{i+1} to t_i, conditioned that in the same time interval the environment coordinates go from z_{i+1} to z_i. The stochastic interpretation of the reduced propagator with stochastic Schrödinger equations is discussed in section (2.5).

Let us show briefly in the following sections how the reduced propagator can be used to compute the most general quantity which characterizes the dynamics of a quantum open system, namely the N-time correlation function of its observables, for different initial conditions of the total system. How to compute the corresponding reduced density matrix is also shown.

2.2.1 Initial decorrelated state $\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0)$

We assume an initially decorrelated state $\rho_{tot}(0) = \rho_s(0) \otimes \rho_B$, where $\rho_s(t_0) = |\psi_0\rangle\langle\psi_0|$ and $\rho_B = |z_0\rangle\langle z_0|/\langle z_0|z_0\rangle$. Let us for instance define the N-time correlation function for a set of observables in Heisenberg representation, $\{A_1(t_1), \cdots, A_N(t_N)\} = \mathbf{A}(\mathbf{t})$ as [2]

$$\begin{aligned} C_{A_1,A_2,\cdots,A_N}(t_1, t_2, \cdots, t_N|\Psi_0) &= C_{\mathbf{A}}(\mathbf{t}|\Psi_0) \\ &= \langle\Psi_0|A_1(t_1)\cdots A_N(t_N)|\Psi_0\rangle, \end{aligned} \tag{2.9}$$

with $t_1 > t_2 > \cdots > t_N$ and $\mathbf{t} = \{t_1, \cdots, t_N\}$. In the partial interaction picture with respect to the environment, the N-time correlation function is given by

$$C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \langle\Psi_0| \prod_{i=1}^{N} \mathcal{U}_I^{-1}(t_i, 0) A_i \mathcal{U}_I(t_i, 0)|\Psi_0\rangle$$

---

[2] We will see in Part (III) MTCF can be defined with a different time ordering.

$$\begin{aligned} &= \langle\Psi_0|\mathcal{U}_I^{-1}(t_1,0)A_1\mathcal{U}_I(t_1,t_2)A_2\mathcal{U}_I(t_2,t_3)\cdots \\ &\quad \mathcal{U}_I(t_{N-1},t_N)A_N\mathcal{U}_I(t_N,t_0)|\Psi_0\rangle \end{aligned} \tag{2.10}$$

where $\mathcal{U}_I(t_1,t_2)$ is the evolution operator of the system in the interaction picture defined in (2.8), and $|\Psi_t\rangle = |\psi_0\rangle|z_0\rangle/\langle z_0|z_0\rangle$. We now chose the Bargmann coherent state basis for the environment whose resolution of the identity is given by

$$1 = \int d\mu(z)|z\rangle\langle z|. \tag{2.11}$$

If we introduce N identity operators (2.11) in (2.10), the correlation function is given by

$$C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \prod_{i=1}^{N}\int d\mu(z_i)\langle\psi_0|G^\dagger(z_0^*z_1|t_0t_1)A_iG(z_i^*z_{i+1}|t_it_{i+1})|\psi_0\rangle. \tag{2.12}$$

For a one-time correlation function (also referred as expectation value) of an observable,

$$\begin{aligned} \langle A_1\rangle = C_{A_1}(t_1|\Psi_0) &= \langle\Psi_0|A_1(t_1)|\Psi_0\rangle \\ &= \int d\mu(z_1)\langle\psi_0|G^\dagger(z_0^*z_1|t_0t_1)A_1G(z_1^*z_0|t_1t_0)|\psi_0\rangle \\ &= \int d\mu(z_1)\sum_{mm'}\langle\psi_0|\times G^\dagger(z_0^*z_1|t_0t_1)|m\rangle\langle m|A_1|m'\rangle \\ &\quad \langle m'|G(z_1^*z_0|t_1t_0)|\psi_0\rangle \\ &= \sum_{m'}\langle m'|\rho_s(t_1t_0|z_0)A_1|m'\rangle, \end{aligned} \tag{2.13}$$

where we have defined

$$\rho_s(t_1t_0|z_0) = \int d\mu(z_1)|\psi_{t_1t_0}(z_1^*z_0)\rangle\langle\psi_{t_1t_0}(z_0^*z_1)|, \tag{2.14}$$

with $|\psi_{t_1t_0}(z_1^*z_0)\rangle = G(z_1^*z_0|t_1t_0)|\psi_0\rangle$ and $\langle\psi_{t_1t_0}(z_0^*z_1)| = \langle\psi_0|G^\dagger(z_0^*z_1|t_0t_1)$, which is the reduced density operator. We have also considered the system closure relation as $1 = \sum_m |m\rangle\langle m|$. Equation (2.13) can be expressed in the usual manner as,

$$C_{A_1}(t_1|\Psi_0) = \langle\Psi_0|A_1(t_1)|\Psi_0\rangle = Tr_S\left(\rho_s(t_1t_0|z_0)A\right), \tag{2.15}$$

or, in terms of $|\psi_{t_1t_0}(z_1^*z_0)\rangle$,

$$C_{A_1}(t_1|\Psi_0) = \int d\mu(z_1)\langle\psi_{t_1t_0}(z_0^*z_1)|A_1|\psi_{t_1t_0}(z_1^*z_0)\rangle. \tag{2.16}$$

With $t_0 = 0$ and $z_0 = 0$, the we obtain the reduced density matrix usually found in the literature [3],

$$\rho_s(t) = \int d\mu(z)|\psi_t(z^*)\rangle\langle\psi_t(z)|, \tag{2.17}$$

and

$$C_{A_1}(t_1|\Psi_0) = \int d\mu(z)\langle\psi_t(z)|A_1|\psi_t(z^*)\rangle. \tag{2.18}$$

---

[3] When only the environmental state z_1 and the time t_1 enters in the equations, we will often denote them just as z and t for simplicity.

Notice that we have simplified the notation by setting $z_1 = z$. These simplifications in the notation are made throughout the whole work whenever it is possible and do not lead to confusion.

Let us now suppose the following initial state for the total system in terms of the coherent state basis

$$\rho_{tot}(t_0) = |\psi_0\rangle\langle\psi_0| \otimes \int d\mu(z_0) P(z_0, z_0^*)|z_0\rangle\langle z_0| \tag{2.19}$$

where $P(z_0, z_0^*)$ is the coherent state diagonal distribution [43, 53] to be chosen for each particular environment [4], and $|\Psi_0\rangle = |\psi_0\rangle||z_0\rangle$ in terms of coherent states $||z_0\rangle$, and $|\Psi_0\rangle = \exp(-|z_0|^2/2)|\psi_0\rangle|z_0\rangle$ in terms of Bargmann coherent states (see Appendix (B)). Then, $\rho_{tot}(0)$ is a decorrelated state, since it can be written as $\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0)$, with $\rho_s(t_0) = |\psi_0\rangle\langle\psi_0|$, and $\rho_B(t_0) = \int d^2z_0 P(z_0, z_0^*)|z_0\rangle\langle z_0|$. We then define the N-time correlations as (2.12), but adding an additional average with respect to the initial distribution $P(z_0, z_0^*)$,

$$\begin{aligned} C_{\mathbf{A}}(\mathbf{t}|\rho_{tot}(t_0)) &= Tr_{tot}\left(A_1(t_1)\cdots A_N(t_N)\rho_{tot}(0)\right) \\ &= \int d\mu(z_0)P(z_0, z_0^*)\langle\psi_0(z_0)|\left(\sum_m |m\rangle\langle m|\right) \\ &\quad \times\langle z_0|\left(\int d\mu(z)|z\rangle\langle z|\right)|A_1(t_1)\cdots A_N(t_N)|z_0\rangle|\psi_0\rangle \\ &= \int d\mu(z)\int d\mu(z_0)P(z_0, z_0^*)\langle\psi_0|\langle z_0|A_1(t_1)\cdots A_N(t_N)\rangle|z_0\rangle|\psi_0\rangle, \end{aligned} \tag{2.20}$$

where we have used the Bargmann unitary relation $\int d\mu(z)|z\rangle\langle z| = 1$, and a basis $\{|m\rangle\}$ for the system with unitary relation $\sum_m |m\rangle\langle m| = 1$ [47, 48].

As before, expectation values can be expressed in terms of the former equation by setting $N = 1$, or in terms of the density operator $\rho_s(t_1, t_0)$, which now is defined in terms of $\rho_{tot}(t_1, t_0) = \mathcal{U}_I(t_1, t_0)\rho_{tot}(t_0)\mathcal{U}_I^{-1}(t_1, t_0)$, with $\rho_{tot}(t_0)$ given by (2.19), as

$$\rho_s(t_1, t_0) = \int d\mu(z_1)\int d\mu(z_0)P(z_0, z_0^*)|\psi_{t_1 t_0}(z_1^* z_0)\rangle\langle\psi_{t_0 t_1}(z_0^* z_1)|, \tag{2.21}$$

where $|\psi_{t_1 t_0}(z_1^* z_0)\rangle = G(z_1^* z_0|t_1 t_0)|\psi_0\rangle$. In the same way, it can be easily verified that with $\rho_{tot}(0)$ given by (2.19), the environmental density operator is just

$$\rho_B(t_0) = Tr_S\left(\rho_{tot}(t_0)\right) = \int d^2z_0 P(z_0, z_0^*)e^{-|z_0|^2}|z_0\rangle\langle z_0|. \tag{2.22}$$

In Section (5.2.1.2) of Chapter (II) we derive an equation thermal master equation for $\rho_s(t)$ (considering for simplicity $t_0 = 0$). Such equation corresponds to a $\rho_{tot}(t_0)$ given by (2.19) with $P(z_0, z_0^*)$ chosen as the coherent P representation of a thermal environment. Analogously, in Appendix (L) we derive evolution equation for two-time correlations in a thermal environment.

It is possible to use other distributions for the environment. If we represent ρ_B in the $R(\alpha, \beta)$ representation of coherent states [43, 53], then we would obtain

$$\rho_B = \int d^2z_0' d\mu(z_0')\int d^2z_0 d\mu(z_0)R(z_0'^*, z_0)|z_0'\rangle\langle z_0|, \tag{2.23}$$

---

[4] Since it is a quantum distribution, $P(z_0, z_0^*)$ can take negative values over a limited range and therefore should not be considered as a probability distribution. Instead, it is often referred to as quasi-distribution function [53]. In the present case, in order to perform the sampling or the analytical sum over the coherent states, it is convenient that P is a positive definite function. This is the case of the P function corresponding to a thermal reservoir, which is one we study in this thesis.

where

$$R(z_0'^*, z_0) = \langle z_0'|\rho_B|z_0\rangle \tag{2.24}$$

Inserting (2.22) in the former expression, one obtains the relation between the P and the R representations,

$$R(z_0'^*, z_0) = e^{-\frac{|z_0'|^2}{2}} e^{-\frac{|z_0|^2}{2}} \int d^2\alpha P(\alpha, \alpha^*) e^{-|\alpha|^2} e^{z_0'^* \alpha} e^{\alpha^* z_0}. \tag{2.25}$$

2.2.2 Initially correlated state $\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0) + \rho_{corr}(t_0)$

2.2.2.1 Pure state We set $\rho_{tot}(t_0) = \int d\mu(z_0) \int d\mu(z_0') |\Psi_0(z_0^*)\rangle\langle\Psi_0(z_0')|$, where

$$|\Psi_0(z_0)\rangle = \langle z_0|\Psi_0\rangle|z_0\rangle = |\psi_0(z_0^*)\rangle|z_0\rangle. \tag{2.26}$$

Then, the MTCF are written in a similar manner as (2.12), but adding two integrals: one over the variable z_0, and another over the variable $z_{N+1} = z_0'$,

$$C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \prod_{i=0}^{N+1} \left[\int d\mu(z_i) \right] \langle\psi_0(z_0)|G^\dagger(z_0^* z_1|t_0 t_1) \prod_{i=1}^{N} A_i G(z_i^* z_{i+1}|t_i t_{i+1})|\psi_0(z_0'^*)\rangle. \tag{2.27}$$

Notice that these two integrals will also be performed over the wave vectors $|\langle\psi_0(z_0)|$ and $|\psi_0(z_0'^*)\rangle$ respectively. The same considerations have to be made in the reduced density operator, that is written like (2.14), but with two additional integrals over z_0 and z_0',

$$\rho_s(t_1 t_0|0) = \int d\mu(z_0) \int d\mu(z_0') \int d\mu(z_1) G(z_1^* z_0'|t_0 t_1)|\psi_0(z_0'^*)\rangle\langle\psi_0(z_0)|G^\dagger(z_0^* z_1|t_0 t_1), \tag{2.28}$$

which is reduced to the following mixture,

$$\rho_s(t_1 t_0|0) = \int d\mu(z_1)|\psi_{t_1,t_0}(z_1^*)\rangle\langle\psi_{t_1,t_0}(z_1)| \tag{2.29}$$

with $|\psi_{t_1,t_0}(z_1^*)\rangle = \int d\mu(z_0) G(z_1^* z_0|t_0 t_1)|\psi_0(z_0^*)\rangle$.

2.2.2.2 Statistical mixture Let us now suppose a mixture for $\rho_{tot}(t_0)$,

$$\rho_{tot}(t_0) = \int d\mu(z_0) \mathcal{J}(z_0, z_0^*) |\Psi_0(z_0^*)\rangle\langle\Psi_0(z_0)|, \tag{2.30}$$

where $\mathcal{J}(z_0, z_0^*)$ is the statistical probability for the member $|\Psi_0(z_0^*)\rangle$ of the statistical ensemble. Notice that this expansion is similar in form to (2.19), but now with $|\psi_0(z_0^*)\rangle|z_0\rangle$, and a different probability distribution (the statistical mixture now is not the environment, but the total system). The N-time correlations are defined as (2.20) but replacing $\langle\psi_0|$ by $\langle\psi_0(z_0)|$, $|\psi_0\rangle$ by $|\psi_0(z_0^*)\rangle$, and $P(z_0, z_0^*)$ by $\mathcal{J}(z_0, z_0^*)$.

$$\begin{aligned} C_{\mathbf{A}}(\mathbf{t}|\rho_{tot}(t_0)) &= Tr_{tot}\left(A_1(t_1) \cdots A_N(t_N)\rho_{tot}(0)\right) \\ &= \int d\mu(z) \int d^2 z_0 \mathcal{J}(z_0, z_0^*) \langle\psi_0(z_0)|\langle z_0|A_1(t_1) \cdots A_N(t_N)\rangle|z_0\rangle|\psi_0(z_0)\rangle, \end{aligned} \tag{2.31}$$

In the same way as (2.21), the reduced density operator is defined as

$$\rho_s(t_1,t_0) = \int d\mu(z_1) \int d\mu(z_0) \mathcal{J}(z_0,z_0^*) |\psi_{t_1t_0}(z_1^* z_0)\rangle\langle\psi_{t_0t_1}(z_0^* z_1)|, \tag{2.32}$$

where $|\psi_{t_1t_0}(z_1^*z_0)\rangle = G(z_1^*z_0|t_1t_0)|\psi_0(z_0^*)\rangle$. The environmental density operator is equal to

$$\begin{aligned}\rho_B(t_1,t_0) &= Tr_S\left(\rho_{tot}(t_1,t_0)\right) = \int d\mu(z_0)\mathcal{J}(z_0,z_0^*)|z_0\rangle\langle z_0| \\ &\times \sum_m \langle m|\mathcal{U}_I(t_1,t_0)|\psi_0(z_0^*)\rangle\langle\psi_0(z_0)|\mathcal{U}_I^{-1}(t_1,t_0)|m\rangle \\ &= \int d\mu(z_0)\mathcal{J}(z_0,z_0^*)\langle\psi_0(z_0)|\psi_0(z_0^*)\rangle|z_0\rangle\langle z_0|. \end{aligned} \tag{2.33}$$

A description of the different elements of the reduced density operator, as well as some of its properties is given in Appendix (C).

Once the evolution equation for the reduced propagators $G(z_i^* z_{i+1}|t_i t_{i+1})$ is known, any quantity of the system (either quantum mean values or multiple-time correlations) can be computed, provided that the sums $\int d\mu(z_i)$ over the coherent state labels can be performed. In the Sections (2.3) and (2.4) we show how to compute the evolution equation for the reduced propagator, while the Section (2.5) is devoted to the problem of how to perform the integrals over the coherent state labels.

2.3 EVOLUTION EQUATION FOR THE REDUCED PROPAGATOR

To proceed further we need to derive the equation of motion of the reduced propagator $G(z_i^* z_{i+1}|t_i t_{i+1})$ [3, 4]. Obviously, once the time evolution of the reduced propagator is obtained, the one corresponding to the vacuum reduced propagator (2.6) follows from the identities $z_{i+1} = t_{i+1} = 0$. Let us consider the following time derivative

$$\frac{\partial G(z_i^* z_{i+1}|t_i t_{i+1})}{\partial t_i} = \left\langle z_i \left| \frac{\partial \mathcal{U}_I(t_i,t_{i+1})}{\partial t_i} \right| z_{i+1} \right\rangle. \tag{2.34}$$

The evolution operator $\mathcal{U}_I(t_i,t_{i+1})$ given by (2.8) satisfies the Schrödinger equation in the partial interaction picture

$$\frac{\partial \mathcal{U}_I(t_i,t_{i+1})}{\partial t_i} = \Big(-iH_S - i\sum_n g_\lambda (L^\dagger a_\lambda e^{-i\omega_\lambda t_i} + L a_\lambda^\dagger e^{i\omega_\lambda t_i}) \Big) \mathcal{U}_I(t_i,t_{i+1}). \tag{2.35}$$

When inserted in (2.34) this equation leads to

$$\begin{aligned}\frac{\partial G(z_i^* z_{i+1}|t_i t_{i+1})}{\partial t_i} = &\Big(-iH_S - iL\sum_\lambda g_\lambda e^{i\omega_\lambda t_i} z_{i,\lambda}^* \Big) G(z_i^* z_{i+1}|t_i t_{i+1}) \\ &-iL^\dagger \sum_\lambda g_\lambda e^{-i\omega_\lambda t_i} \langle z_i|a_\lambda \mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle, \end{aligned} \tag{2.36}$$

where we have used the property $\langle z|a_\lambda^\dagger = \langle z|z_\lambda^*$. To proceed further it is convenient to treat the matrix element $\langle z_i|a_\lambda\mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle$ that equals to $\langle z_i|\mathcal{U}_I(t_i,t_{i+1})a_\lambda(t_i,t_{i+1})|z_{i+1}\rangle$, with $a_\lambda(t_i,t_{i+1}) = \mathcal{U}_I^{-1}(t_i,t_{i+1})a_\lambda\mathcal{U}_I(t_i,t_{i+1})$. Integrating the Heisenberg equations of motion for $a_\lambda(t_i,t_{i+1})$,

$$\frac{d}{dt_i} a_\lambda(t_i,t_{i+1}) = i\omega_\lambda a_\lambda(t_i,t_{i+1})$$

$$\begin{aligned}&+\ i\left[H_S+H_B+\sum_\lambda g_\lambda\left(a_\lambda L^\dagger e^{i\omega_\lambda t_{i+1}}+La_\lambda e^{-i\omega_\lambda t_{i+1}}\right),a_\lambda(t_i,t_{i+1})\right]=\\ &-\ ig_\lambda e^{-i\omega_\lambda t_i}L(t_i,t_{i+1}),\end{aligned}\tag{2.37}$$

with $[A,B]=AB-BA$, it follows

$$a_\lambda(t_i,t_{i+1})=a_\lambda(t_{i+1},t_{i+1})-ig_\lambda\int_{t_{i+1}}^{t_i}d\tau L(\tau,t_{i+1})e^{i\omega_\lambda\tau},\tag{2.38}$$

with

$$L(t_i,t_{i+1})=e^{iH_Bt_{i+1}}e^{-iH_{tot}(t_{i+1}-t_i)}Le^{iH_{tot}(t_{i+1}-t_i)}e^{-iH_Bt_{i+1}}.\tag{2.39}$$

Gathering the results, the equation (2.36) becomes

$$\begin{aligned}\frac{\partial G(z_i^*z_{i+1}|t_it_{i+1})}{\partial t_i}&=\big(-iH_S+Lz_{i,t_i}^*-L^\dagger z_{i+1,t_i}\big)G(z_i^*z_{i+1}|t_it_{i+1})\\ &-\ L^\dagger\int_{t_{i+1}}^{t_i}d\tau\alpha(t_i-\tau)\langle z_i|\mathcal{U}_I(t_i,t_{i+1})L(\tau,t_{i+1})|z_{i+1}\rangle,\end{aligned}\tag{2.40}$$

where we defined the functions

$$z_{i,t}=i\sum_\lambda g_\lambda z_{i,\lambda}e^{-i\omega_\lambda t},\tag{2.41}$$

and

$$\alpha(t-\tau)=\sum_\lambda|g_\lambda|^2e^{-i\omega_\lambda(t-\tau)}.\tag{2.42}$$

The function $z_{i,t}$ is a sum over time dependent coherent states and $\alpha(t-\tau)$ is its time autocorrelation function, as it can be easily verified by computing the average $\mathcal{M}[z_{i,t}z_{i,\tau}^*]$ with respect to the measure $d\mu(z_i)=\prod(d^2z_{i_\lambda}\exp(-|z_{i,\lambda}|^2)/\pi$. The function $\alpha(t-\tau)$ is the environmental correlation function introduced in Chapter (1). In terms of the spectral function $J(\omega)$ and for zero temperature is (1.50)

$$\alpha(t-\tau)=\int d\omega J(\omega)e^{-i\omega(t-\tau)},\tag{2.43}$$

from where it can be inferred that effectively $J(\omega)=\sum_\lambda|g_\lambda|^2\delta(\omega-\omega_\lambda)$. We can now see from equation (2.40) why the environmental function is responsible of the dependence of the evolution of the system over its past history, being the kernel of an integral term from the initial time t_{i+1} to the actual time t_i. The last equation can be written in a different manner by noting that

$$\langle z_i|\mathcal{U}_I(t_i,t_{i+1})L(\tau,t_{i+1})|z_{i+1}\rangle=\frac{\delta G(z_i^*z_{i+1}|t_it_{i+1})}{\delta z_{i,\tau}^*},\tag{2.44}$$

as derived in Appendix (K), so that equation (2.40) becomes

$$\begin{aligned}\frac{\partial G(z_i^*z_{i+1}|t_it_{i+1})}{\partial t_i}&=\big(-iH_S+Lz_{i,t_i}^*-L^\dagger z_{i+1,t_i}\big)G(z_i^*z_{i+1}|t_it_{i+1})\\ &-L^\dagger\int_{t_{i+1}}^{t_i}d\tau\alpha(t_i-\tau)\frac{\delta G(z_i^*z_{i+1}|t_it_{i+1})}{\delta z_{i,\tau}^*}.\end{aligned}\tag{2.45}$$

From equation (2.40) (or its equivalent version (2.45)), we could integrate the reduced propagators with the initial conditions $G(z_i^*z_{i+1}|t_it_i)=\exp\left(z_i^*z_{i+1}\right)$. However, the time dependency of the operator appearing in the last term of (2.40), $L(\tau, t_{i+1}) = \mathcal{U}_I^{-1}(\tau, t_{i+1}) L \mathcal{U}_I(\tau, t_{i+1})$, with $\mathcal{U}_I(\tau, t_{i+1})$ given by (2.8), is over the total Hamiltonian operator, so that equation (2.40) is still not a closed equation over the reduced Hilbert space of the system, and it is just a particular representation of the Schrödinger equation for the system and the environment.

If we want to express the last term of equation (2.40) as an object in the system Hilbert space without the use of any approximation, it is necessary to do the following

$$\begin{aligned} \langle z_i \mid \mathcal{U}_I(t_i, \tau) L \mathcal{U}_I(\tau, t_{i+1}) \mid z_{i+1} \rangle &= \mathcal{M}_l \big[\langle z_i \mid \mathcal{U}_I(t_i, \tau) \mid z_l \rangle L \langle z_l \mid \mathcal{U}_I(\tau, t_{i+1}) \mid z_{i+1} \rangle \big] \\ &= \mathcal{M}_l \big[G(z_i^* z_l | t_i \tau) L G(z_l^* z_{i+1} | \tau t_{i+1}) \big], \end{aligned} \tag{2.46}$$

where in the second line we have inserted $\mathit{1} = \int \frac{d^2 z}{\pi} e^{-|z|^2} |z\rangle\langle z|$, and we have defined

$$\mathcal{M}_l[\cdots] = \int d\mu(z_l) \cdots . \tag{2.47}$$

In that notation, equation (2.40) can be written as

$$\begin{aligned} \frac{\partial G(z_i^* z_{i+1} | t_i t_{i+1})}{\partial t_i} &= \big(- i H_S + L z_{i,t_i}^* - L^\dagger z_{i+1,t_i} \big) G(z_i^* z_{i+1} | t_i t_{i+1}) \\ &\quad - L^\dagger \int_{t_{i+1}}^{t_i} d\tau \alpha(t_i - \tau) \mathcal{M}_l \left[G(z_i^* z_l | t_i \tau) L G(z_l^* z_{i+1} | \tau t_{i+1}) \right]. \end{aligned} \tag{2.48}$$

In this equation, the last term expresses how the dissipation at time t depends on previous trajectories of other system propagators [49].

In the next section we discuss some schemes and approximations to compute this last term in order to express it as a function of the reduced propagator belonging to the system Hilbert space, which makes (2.40) an explicit equation for the reduced propagator.

2.4 CLOSED FORM FOR THE EVOLUTION EQUATION OF THE REDUCED PROPAGATOR

It is not always possible to compute exactly the matrix element $\langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle$, and to express it as a function of the reduced propagator.

As previously noted, only in very exceptional cases this can be done. Particularly, when $L(\tau, t_{i+1}) \propto H_S(\tau, t_{i+1})$, then $[L, H_{tot}] = 0$ and therefore $H_S(\tau, t_{i+1}) = H_S$, so that

$$\langle z_i | L(\tau, t_i) \mathcal{U}_I(t_i, t_{i+1}) | z_{i+1} \rangle \propto H_S G(t_i t_{i+1} | z_i^* z_{i+1}). \tag{2.49}$$

For the particular case $H_S = \omega_s \sigma_z / 2$, the choice $L = \sigma_z$ represents a *solvable model* that will serve in next chapters to derive analytical expressions for the evolution of quantum mean values and multiple-time correlation functions of system observables.

For other choices of L some approximate scheme has to be taken. We shall focus on the weak coupling assumption and the near Markovian limit. We start by discussing in Section (2.4.1) a method to derive an approximate solution based on assuming, as an ansatz, that the coupling operator $L(\tau, t_{i+1})$ can be expanded in a certain way. This method is based on a procedure proposed by Cresser in [70], and gives similar results as the consistency condition proposed in [40]. Other approximations are discussed in Sections (2.4.2), (2.4.3) and (2.4.4). In all these schemes, the idea is to express the matrix element as a certain system operator $O(z_{i+1} z_i^*, t, \tau)$ multiplied by the propagator,

$$\begin{aligned} \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle &= \langle z_i | L(\tau, t_i) \mathcal{U}_I(t_i, t_{i+1}) | z_{i+1} \rangle \\ &= O(z_{i+1} z_i^*, t, \tau) G(z_i^* z_{i+1} | t_i t_{i+1}) \end{aligned} \tag{2.50}$$

where the operator O is constructed in an approximate manner. Following the relation (2.44), the former expression is equivalent to

$$\frac{\delta G(z_i^* z_{i+1}|t_i t_{i+1})}{\delta z_{i,\tau}^*} = O(z_{i+1} z_i^*, t, \tau) G(z_i^* z_{i+1}|t_i t_{i+1}) \tag{2.51}$$

The last expression was proposed in [40, 54] for the evolution equation of vacuum propagators (2.6). Inserting (2.50) in (2.40), we get the following closed evolution equation for the general reduced propagator,

$$\begin{aligned} \frac{\partial G(z_i^* z_{i+1}|t_i t_{i+1})}{\partial t_i} &= \big(-iH_S + L z_{i,t_i}^* - L^\dagger z_{i+1,t_i} \big) G(z_i^* z_{i+1}|t_i t_{i+1}) \\ &- L^\dagger \int_{t_{i+1}}^{t_i} d\tau \alpha(t_i - \tau) O(z_{i+1} z_i^*, t, \tau) G(z_i^* z_{i+1}|t_i t_{i+1}). \end{aligned} \tag{2.52}$$

The *open equation* (2.40) is used in Chapter (8) to derive a theory of MTCF without the use of any approximation. Because the open structure of the reduced propagators, N-time correlations are found to depend on $N+1$-time correlations. When a perturbative hypothesis is assumed, the *hierarchy* is used to derive N-time correlation functions up to second order in the coupling parameter.

The *closed equation* (2.52) is used,

- As a second order equation in the coupling parameter, in Part (II) to derive a second order master equation, and in Part (III) to get N-time correlation functions up to the same order.
- As an equation obtained within the expansion assumption, for $L = \sigma_{12}$ and initial vacuum state for the environment, in Part (IV) for the two level atom coupled to the radiation field of a PBG.
- As an exact model for $L = \sigma_z$ and general z_{i+1}, also referred as *solvable model*, in Chapter (9) to compute two-time correlation functions.

2.4.1 Expansion assumption and consistency condition

The coupling operator appearing in (2.40) can be expressed in the following way as an ansatz [70],

$$L(\tau, t_{i+1}) = \sum_\alpha F_\alpha(\tau, t_i, \{a_\lambda\}) S_\alpha(t_i, t_{i+1}), \tag{2.53}$$

where the set $\{S_i\}$ represent a basis of system operators, and $F_\alpha(\tau, t_i, \{a_\lambda\})$ is a certain set of operators of the total Hilbert space[5]. The replacement of the last expression in the matrix element of the last term of (2.40) gives the following formal expression

$$\begin{aligned} \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle &= \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) \left(\sum_\alpha F_\alpha(\tau, t_i, \{a_\lambda\}) S_\alpha(t_i, t_{i+1}) \right) | z_{i+1} \rangle \\ &= \mathcal{F}(t_i, \tau, [z_{i+1}]) \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) | z_{i+1} \rangle \end{aligned} \tag{2.54}$$

where we have defined the following functional of z_{i+1} [6],

$$\mathcal{F}(t_i, \tau, [z_{i+1}]) = \sum_\alpha f_\alpha(\tau, t_i, [z_{i+1}]) S_\alpha. \tag{2.55}$$

---

[5] Notice that F_α does not depend on $a^\dagger$, since in the Heisenberg equation of L such term would correspond to $[L, L]a^\dagger = 0$. This is more clearly seen with the examples we discuss later in this section.

[6] The object $\mathcal{F}(t_i, \tau, [z_{i+1}])$ depends on the environmental coordinates z_{i+1} through the function $z_{i+1,\tau - t_{i+1}}$, defined in (2.41).

The $f_\alpha(\tau, t_i, [z_{i+1}])$ are also functionals obtained by considering $F_\alpha(\tau, t_i, \{a_\lambda\})|z_{i+1}\rangle = |z_{i+1}\rangle f_\alpha(\tau, t_i, [z_{i+1}])$. The evolution equation for each function of the expansion is computed taking into account the Heisenberg equation of $L(\tau, t_{i+1})$, so that

$$\begin{aligned} \frac{d}{d\tau}L(\tau, t_{i+1}, \{a_\lambda\})|z_{i+1}\rangle &= \sum_\alpha \left(\frac{d}{d\tau}f_\alpha(\tau, t_i, [z_{i+1}])\right) S_\alpha(t_i, t_{i+1})|z_{i+1}\rangle \\ &= -i\,[H_{tot}, L(\tau, t_{i+1})]\,|z_{i+1}\rangle \end{aligned} \tag{2.56}$$

However, not in all cases can the system of equations for $\{f_\alpha\}$ be solved. First of all, applying the vector $|z_{i+1}\rangle$ simplifies considerably the problem, but only for vacuum reduced propagators, i.e. when $z_{i+1} = 0$, and for particular couplings L. Specifically, when L is a member of the atomic basis of matrices (for instance $\{\sigma_{12}, \sigma_{21}, \sigma_{11}\}$ for a two level atom[7]), the problem is exact. Let us show this in more detail with some examples.

Suppose first that $L = \sigma_{12}$. Notice that this case is quite useful, since it corresponds to an atom dipolarly coupled to an electromagnetic field, or to a Bose-Einstein condensate with an output coupling. Then, considering that for any system operator S the time dependencies are such that $S_\alpha(t_i, t_{i+1}) = \mathcal{U}_I^{-1}(t_i, t_{i+1})S_\alpha\mathcal{U}_I(t_i, t_{i+1})$, with the evolution operators given by (2.8), the evolution equation of each member of the basis and for the Hamiltonian (2.1) are

$$\begin{aligned} \frac{d\sigma_{12}(\tau, t_{i+1})}{d\tau} &= i\omega_S\sigma_{12}(\tau, t_{i+1}) - \sigma_z(\tau, t_{i+1})\nu(\tau) \\ &- \int_{t_{i+1}}^{\tau} dl\alpha(\tau - l)\sigma_z(\tau, t_{i+1})\sigma_{12}(l, t_{i+1}); \\ \frac{d\sigma_{21}(\tau, t_{i+1})}{d\tau} &= -i\omega_S\sigma_{21}(\tau, t_{i+1}) - \nu^\dagger(\tau)\sigma_z(\tau, t_{i+1}) \\ &- \int_{t_{i+1}}^{\tau} dl\alpha^*(\tau - l)\sigma_{21}(l, t_{i+1})\sigma_z(\tau, t_{i+1}); \\ \frac{d\sigma_z(\tau, t_{i+1})}{d\tau} &= 2\sigma_{21}(\tau, t_{i+1})\nu(\tau) + \int_{t_{i+1}}^{\tau} dl\alpha(\tau - l)\sigma_{12}(\tau, t_{i+1})\sigma_{21}(l, t_{i+1}) \\ &+ 2\nu^\dagger(\tau)\sigma_{12}(\tau, t_{i+1}) + \int_{t_{i+1}}^{\tau} dl\alpha^*(\tau - l)\sigma_{21}(l, t_{i+1})\sigma_{12}(\tau, t_{i+1}), \end{aligned} \tag{2.57}$$

with

$$\begin{aligned} \nu^\dagger(t) &= -i\sum_\lambda g_\lambda a_\lambda^\dagger(0)e^{i\omega_\lambda t} \\ \nu(t) &= i\sum_\lambda g_\lambda a_\lambda(0)e^{-i\omega_\lambda t}. \end{aligned} \tag{2.58}$$

Let us now consider the matrix element of the open equation (2.40), $\langle z_i|\mathcal{U}_I(t_i, t_{i+1})L(\tau, t_{i+1})|z_{i+1}\rangle$. For the moment we will suppose $z_{i+1} \neq 0$. Considering $L(\tau, t_{i+1}) = \sigma_{12}(\tau, t_{i+1})$, we have

$$\begin{aligned} \frac{d\sigma_{12}(\tau, t_{i+1})}{d\tau}|z_{i+1}\rangle &= i\omega_S\sigma_{12}(\tau, t_{i+1})|z_{i+1}\rangle - \sigma_z(\tau, t_{i+1})z_{i+1,\tau - t_{i+1}}|z_{i+1}\rangle \\ &- \int_{t_{i+1}}^{\tau} dl\alpha(\tau - l)\sigma_z(\tau, t_{i+1})\sigma_{12}(l, t_{i+1})|z_{i+1}\rangle, \end{aligned} \tag{2.59}$$

---

[7] There should be four elements in the basis of a two-level atom. However, since the trace of the density matrix, i.e. the sum of occupation probabilities of all the two levels has to be one, $\sigma_{22}(t) = 1 - \sigma_{11}(t)$ at any time t.

where $z_{i+1,\tau-t_{i+1}} = i\sum_{\lambda} g_{\lambda} z_{i+1} e^{i\omega_{\lambda}(\tau-t_{i+1})}$. Now we consider the aforementioned expansion of $\sigma_{12}(l, t_{i+1})$ in terms of the basis matrices,

$$\sigma_{12}(l,t_{i+1}) = f_1(l,\tau)\sigma_{11}(\tau,t_{i+1}) + f_2(l,\tau)\sigma_{12}(\tau,t_{i+1}) + f_3(l,\tau)\sigma_{21}(\tau,t_{i+1}), \tag{2.60}$$

which replaced in (2.59) gives rise to the following result

$$\begin{aligned}
\frac{d\sigma_{12}(\tau,t_{i+1})}{d\tau}|z_{i+1}\rangle &= i\omega_S\sigma_{12}(\tau,t_{i+1})|z_{i+1}\rangle - (1-2\sigma_{11}(\tau,t_{i+1}))z_{i+1,\tau-t_{i+1}}|z_{i+1}\rangle \\
&- \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)(1-2\sigma_{11}(\tau,t_{i+1}))\Big\{f_1(l,\tau)\sigma_{11}(\tau,t_{i+1}) \\
&+ f_2(l,\tau)\sigma_{12}(\tau,t_{i+1}) + f_3(l,\tau)\sigma_{21}(\tau,t_{i+1})\Big\}|z_{i+1}\rangle, \qquad (2.61)
\end{aligned}$$

where we have also considered $\sigma_z(\tau,t_{i+1}) = (1-2\sigma_{11}(\tau,t_{i+1}))$. Simplifying and ordering the last expression, we get

$$\begin{aligned}
\frac{d\sigma_{12}(\tau,t_{i+1})}{d\tau}|z_{i+1}\rangle &= z_{i+1,\tau-t_{i+1}}|z_{i+1}\rangle \\
&- \left(\int_{t_{i+1}}^{\tau} \alpha(\tau-l)f_1(l,t_{i+1}) + 2z_{i+1,\tau-t_{i+1}}\right)\sigma_{11}(\tau,t_{i+1})|z_{i+1}\rangle \\
&+ \left(i\omega_S - \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_2(l,t_{i+1})\right)\sigma_{12}(\tau,t_{i+1})|z_{i+1}\rangle \\
&+ \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_3(l,t_{i+1})\sigma_{21}(\tau,t_{i+1}). \qquad (2.62)
\end{aligned}$$

To proceed further, it is necessary to replace in (2.62) the expansion of all the basis operators $\{\sigma_{j,k}\}(\tau,t_{i+1})$, with $j,k = 1,\cdots 3$ in terms of the functions $\{f_{\alpha}(\tau,t_{i+1})\}$ where $\alpha = 1,2,3$, which according to (2.60) is,

$$\begin{aligned}
\sigma_{21}(\tau,t_{i+1}) &= \sigma_{12}^{*}(\tau,t_{i+1}) = f_1^{*}(\tau,t_{i+1})\sigma_{11}(t_{i+1},t_{i+1}) + f_2^{*}(\tau,t_{i+1})\sigma_{21}(t_{i+1},t_{i+1}) \\
&+ f_3^{*}(\tau,t_{i+1})\sigma_{21}(t_{i+1},t_{i+1}) \\
\sigma_{11}(\tau,t_{i+1}) &= \sigma_{12}(\tau,t_{i+1})\sigma_{21}(\tau,t_{i+1}) = |f_3(\tau,t_{i+1})|^2 \\
&+ \left(|f_1(\tau,t_{i+1})|^2 + |f_2(\tau,t_{i+1})|^2 - |f_3(\tau,t_{i+1})|^2\right)\sigma_{11}(t_{i+1},t_{i+1}) \\
&+ f_1(\tau,t_{i+1})f_3^{*}(\tau,t_{i+1})\sigma_{12}(t_{i+1},t_{i+1}) + f_3(\tau,t_{i+1})f_1^{*}(\tau,t_{i+1})\sigma_{21}(t_{i+1},t_{i+1}) \qquad (2.63)
\end{aligned}$$

Note that $S_{\alpha}(t_{i+1},t_{i+1}) = S_{\alpha}(0) = S_{\alpha}$. Inserting (2.63) in (2.62), we find

$$\begin{aligned}
&\frac{d\sigma_{12}(\tau,t_{i+1})}{d\tau}|z_{i+1}\rangle = z_{i+1,\tau-t_{i+1}}|z_{i+1}\rangle - \left(\int_{t_{i+1}}^{\tau} \alpha(\tau-l)f_1(l,t_{i+1}) + 2z_{i+1,\tau-t_{i+1}}\right)\Big\{|f_3(\tau,t_{i+1})|^2 \\
+ &\left(|f_1(\tau,t_{i+1})|^2 + |f_2(\tau,t_{i+1})|^2 - |f_3(\tau,t_{i+1})|^2\right)\sigma_{11} \\
+ &f_1(\tau,t_{i+1})f_3^{*}(\tau,t_{i+1})\sigma_{12} + f_3(\tau,t_{i+1})f_1^{*}(\tau,t_{i+1})\sigma_{21}\Big\}|z_{i+1}\rangle \\
+ &\left(i\omega_S - \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_2(l,t_{i+1})\right)\Big\{f_1(\tau,t_{i+1})\sigma_{11} + f_2(\tau,t_{i+1})\sigma_{12} + f_3(\tau,t_{i+1})\sigma_{12}\Big\}|z_{i+1}\rangle \\
+ &\int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_3(l,t_{i+1})\Big\{f_1^{*}(\tau,t_{i+1})\sigma_{11} + f_2^{*}(\tau,t_{i+1})\sigma_{21} + f_3^{*}(\tau,t_{i+1})\sigma_{21}\Big\}|z_{i+1}\rangle. \qquad (2.64)
\end{aligned}$$

On the other hand, the time derivative with respect to τ of $\sigma_{12}(\tau, t_{i+1})$ expanded in the basis operators has the same form as (2.56) but projected over $|z_{i+1}\rangle$, so that

$$\begin{aligned}\frac{d\sigma_{12}(\tau,t_{i+1})}{d\tau}|z_{i+1}\rangle &= \frac{df_1(\tau,t_{i+1})}{d\tau}\sigma_{11}|z_{i+1}\rangle + \frac{df_2(\tau,t_{i+1})}{d\tau}\sigma_{12}|z_{i+1}\rangle \\ &+ \frac{df_3(\tau,t_{i+1})}{d\tau}\sigma_{21}|z_{i+1}\rangle. \end{aligned} \tag{2.65}$$

Rearranging (2.64) and comparing with (2.65), we get the following system of equations,

$$\begin{aligned}
& 2z_{i+1,\tau-t} - \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)|f_3(\tau,t_{i+1})|^2 - 2z_{i+1,\tau-t}|f_3(\tau,t_{i+1})|^2 = 0; \\
& \frac{df_1(\tau,t_{i+1})}{d\tau} = -\left(\int_{t_{i+1}}^{\tau} \alpha(\tau-l)f_1(l,t_{i+1}) + 2z_{i+1,\tau-t_{i+1}}\right) \\
& \left(|f_1(\tau,t_{i+1})|^2 + |f_2(\tau,t_{i+1})|^2 - |f_3(\tau,t_{i+1})|^2\right) \\
+ & \left(i\omega_S - \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_2(l,t_{i+1})\right) f_1(\tau,t_{i+1}) \\
+ & \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_3(l,t_{i+1})f_1^*(\tau,t_{i+1}); \\
& \frac{df_2(\tau,t_{i+1})}{d\tau} = f_1(\tau,t_{i+1})f_3^*(\tau,t_{i+1}) \\
+ & \left(i\omega_S - \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_2(l,t_{i+1})\right) f_2(\tau,t_{i+1}) \\
+ & \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_3(l,t_{i+1})f_3^*(\tau,t_{i+1}); \\
& \frac{df_3(\tau,t_{i+1})}{d\tau} = f_3(\tau,t)f_1^*(\tau,t) \\
+ & \left(i\omega_S - \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_2(l,t_{i+1})\right) f_3(\tau,t_{i+1}) \\
+ & \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_3(l,t_{i+1})f_2^*(\tau,t_{i+1}).
\end{aligned} \tag{2.66}$$

From (2.60) the initial conditions for the system are such that $f_1(t_{i+1}, t_{i+1}) = f_3(t_{i+1}, t_{i+1}) = 0$ and $f_2(t_{i+1}, t_{i+1}) = 1$. The former system is quite complicated to solve, since the terms of the evolution equations are themselves the functions that are being evolved, but in a domain where they have not already been calculated. To our knowledge, the only way to obtain an easy solution is to set $z_{i+1} = 0$, so that the functions $f_1(\tau, 0) = f_3(\tau, 0) = 0$, and there is only one equation left

$$\frac{df_2(\tau,t_{i+1})}{d\tau} = \left(i\omega_S - \int_{t_{i+1}}^{\tau} dl\alpha(\tau-l)f_2(l,t_{i+1})\right) f_2(\tau,t_{i+1}). \tag{2.67}$$

In that case, the matrix element

$$\langle z_i|\mathcal{U}_I(t_i,t_{i+1})\sigma_{12}(\tau,t_{i+1})|0\rangle = \langle z_i|\sigma_{12}(\tau,t_i)\mathcal{U}_I(t_i,t_{i+1})|0\rangle = f_2(\tau,t_i)\sigma_{12}G(t_it_{i+1}|z_i^*0). \tag{2.68}$$

A similar process can be followed for the case $L(\tau, 0) = \sigma_{21}$, in which case the solution is

$$\langle z_i|\sigma_{21}(\tau, t_i)\mathcal{U}_I(t_i, t_{i+1})|0\rangle = f_2^*(\tau, t_i)\sigma_{21}G(t_it_{i+1}|z_i^*0). \tag{2.69}$$

Notice that for $L = \sigma_{12}, \sigma_{21}, \sigma_z$, the functional (2.55) becomes an operator $\mathcal{F}(t_i, \tau, [z_{i+1}]) = O(t_i, \tau)$.

Before ending this section, it is worth mentioning that for vacuum propagators there exists another possibility which for the choices of L above discussed gives the same results as the last derivation. It consists in assuming (2.51) as an ansatz, and then determining the operator O from the so-called *consistency condition* [40],

$$\frac{d}{dt}\frac{\delta \mid \psi_t(z^*)\rangle}{\delta z_\tau^*} = \frac{\delta}{\delta z_\tau^*}\frac{d \mid \psi_t(z^*)\rangle}{dt}. \tag{2.70}$$

With this considerations, the evolution equation for several systems, like a quantum brownian motion model (in which $L = q$, and q is the position coordinate of the particle), and a simple harmonic oscillator at zero and finite temperature (with $L = a$, with a its annihilation operator) can be obtained (see for instance [40, 55]).

The consistency condition has been also used by Gambetta and Wiseman in [94] to derive a perturbative approach for non-Markovian SSE. Nevertheless, their derivation is only valid for baths at $T = 0$. In the next section we discuss in detail a different perturbative expansion, which is the one used in this thesis.

2.4.2 Weak coupling assumption

The method proposed in this section consists in expanding the element $L(\tau, t_i, \{a_\lambda\}) \equiv L(\tau, t_i)$ of (2.53) in powers of a small coupling parameter g. Such parameter defines the difference in magnitude between the interaction Hamiltonian, H_I, and the so-called free term of the Hamiltonian $H_0 = H_S + H_B$, in such a way that $g[H_0] = [H_I]$ (where $[A]$ denotes the magnitude of A). The derivation followed here is based on the one proposed in [54] for the case of a vacuum propagator (i.e. with $z_{i+1} = 0$). It is clear from (2.54), that the perturbative expansion of L is equivalent to an expansion of O,

$$O(z_{i+1}z_i^*, t, \tau) = \sum_{n=0} g^n O_n(z_{i+1}z_i^*, t, \tau). \tag{2.71}$$

Let us remind the definition of $L(\tau, t_i)$,

$$L(t_i, \tau) = e^{iH_Bt_i}e^{-i(H_S+H_B+H_I)(t_i-\tau)}Le^{i(H_S+H_B+H_I)(t_i-\tau)}e^{-iH_Bt_i}, \tag{2.72}$$

that can be written as

$$L(t_i, \tau) = e^{iH_Bt_i}\mathcal{L}(\tau - t_i)e^{-iH_Bt_i}, \tag{2.73}$$

as a function of an operator $\mathcal{L}(-t)$ that corresponds to a backward Heisenberg propagation

$$\mathcal{L}(-t) = e^{-iH_{tot}t}Le^{iH_{tot}t}. \tag{2.74}$$

This propagator can be formally integrated as

$$\mathcal{L}(-t) = V_{-t}L - ig\int_0^t d\tau e^{-i(H_S+H_B)t}[H_I, V_{-\tau}L]e^{i(H_S+H_B)t} \tag{2.75}$$

where we have defined V_t as a Liouville superoperator such that

$$V_{-t}L = e^{-iH_0t}Le^{iH_0t} = e^{-iH_St}Le^{iH_St}. \tag{2.76}$$

It is important to note that while $V_{-t}L$ is already an operator of the Hilbert space of the system, $\mathcal{L}(-t)$ still acts over the total Hilbert space. Inserting (2.75) into (2.73), we get the zero order of the expansion of $L(t_i, \tau)$

$$\begin{aligned} L(t_i - \tau) &= e^{iH_B t_i} V_{\tau - t_i} L e^{iH_B t_i} - ig e^{iH_B \tau'} \int_0^{t_i - \tau} d\tau' e^{-iH_S(t_i - \tau - \tau')} \\ &\times [H_I, \mathcal{L}(-\tau')] e^{iH_S(t_i - \tau - \tau')} e^{-iH_B \tau'}. \end{aligned} \quad (2.77)$$

In order to extract the first order, it is necessary to replace in the last expression the first term of the expansion (2.75) of $\mathcal{L}(-\tau') = V_{-\tau}L + \mathcal{O}(g)$. In that way, and after replacing the form (2.1) for H_I, we get

$$\begin{aligned} L(t_i - \tau) &= V_{\tau - t_i} L \\ &- i \sum_\lambda g_\lambda \int_0^{t_i - \tau} d\tau' e^{-iH_S(t_i - \tau - \tau')} \Big\{ a_\lambda^\dagger e^{i\omega_\lambda \tau'} [L^\dagger, V_{-\tau}L] \\ &+ [L, V_{-\tau}L^\dagger] a_\lambda e^{-i\omega_\lambda \tau'} \Big\} e^{iH_S(t_i - \tau - \tau')} + \mathcal{O}(g^2) \end{aligned} \quad (2.78)$$

Inserting the last expression in (2.53), we get the following form for the operator O,

$$\begin{aligned} O(z_{i+1} z_i^*, t, \tau) &= V_{\tau - t_i} L + \int_0^{t_i - \tau} d\tau' \left\{ z_{i,\tau'}^* V_{\tau + \tau' - t_i} \{[L^\dagger, V_{-\tau}L]\} \right. \\ &\left. - z_{i+1,\tau'} V_{\tau + \tau' - t_i} \{[L, V_{-\tau}L^\dagger]\} \right\} + \mathcal{O}(g^2), \end{aligned} \quad (2.79)$$

where we the functions $z_{i,\tau'}^*$ and $z_{i,\tau'}^*$ are defined according to (2.41), and $V_{\tau+\tau'-t_i}\{\cdots\}$ acts on all the operators inside the brackets. Inserting the last expression in (2.52) we obtain an equation for the reduced propagator up to the third order in the perturbation parameter. For the applications studied in this work we will just use the second order equation, for which only the first term in (2.79) is needed.

2.4.3 Near Markov approximation

In this approximation, the element $L(\tau, t_{i+1})$ is expanded in a time series in parameter $(t_{i+1} - \tau)$, which is modulated by the time in which the correlation function appearing as an integrand of the last term in (2.40) decays. Since this is the so-called correlation time τ_c, this means that $(t_{i+1} - \tau) \sim \tau_c$. Let us take the matrix element

$$\langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle = \langle z_i | L(\tau, t_i) \mathcal{U}_I(t_i, t_{i+1}) | z_{i+1} \rangle \quad (2.80)$$

and perform an expansion of $L(\tau, t_i) = L(\tau - t_i)$ in Taylor series arround $t_i = \tau$,

$$\begin{aligned} L(\tau - t_i) &= L + \left. \frac{dL(\tau - t_i)}{dt_i} \right|_{t_i = \tau} (t_i - \tau) \\ &+ \frac{d^2 L(\tau - t_i)}{dt_i^2} (t_i - \tau)^2 + \mathcal{O}((t_i - \tau)^3). \end{aligned} \quad (2.81)$$

Let us keep just the first order of the last expansion. From the Heisenberg equation for $L(\tau - t_i)$, we have

$$\left. \frac{dL(\tau - t_i)}{d\tau} \right|_{\tau = t_i} = -i[H_S, L] - i[L^\dagger, L] \sum_\lambda g_\lambda a_\lambda e^{-i\omega_\lambda t_i}, \quad (2.82)$$

that replaced in (2.81) gives the following value for the matrix element (2.80),

$$\begin{aligned}\langle z_i|L(\tau,t_i)\mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle &= LG(z_i^* z_{i+1}|t_it_{i+1}) - i[H_S,L]G(z_i^* z_{i+1}|t_it_{i+1})(t_i-\tau)\\ &- i[L^\dagger,L]\sum_\lambda g_\lambda e^{-i\omega_\lambda t_i}\langle z_i|a_\lambda \mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle(t_i-\tau) + \mathcal{O}((t_i-\tau)^3). \end{aligned} \tag{2.83}$$

To proceed further, it is necessary to calculate the element $\langle z_i|a_\lambda\mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle$. As before, it is only necessary to consider that it is equal to $\langle z_i|\mathcal{U}_I(t_i,t_{i+1})a_\lambda(t_i,t_{i+1})|z_{i+1}\rangle$, where $a_\lambda(t_i,t_{i+1})$ is given by (2.38). Hence,

$$\langle z_i|a_\lambda\mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle = z_{i+1,\lambda} - ig_\lambda\int_{t_{i+1}}^{t_i} d\tau e^{-i\omega_\lambda\tau}\langle z_i \mid L(\tau,t_i)\mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle. \tag{2.84}$$

Considering an expansion of the operator $L(\tau,t_i)$ appearing in (2.81) up to zero order, we have an expansion of the last expression up to such order

$$\langle z_i|a_\lambda\mathcal{U}_I(t_i,t_{i+1})|z_{i+1}\rangle = z_{i+1,\lambda} - ig_\lambda\int_{t_{i+1}}^{t_i} d\tau e^{-i\omega_\lambda\tau}LG(z_i^* z_{i+1}|t_it_{i+1}) + \mathcal{O}((t_i-\tau)), \tag{2.85}$$

which can be inserted in (2.83) to obtain a term of order $(t_i-\tau)$. Therefore, the equation for the propagator is, up to first order,

$$\begin{aligned}\frac{\partial G(z_i^* z_{i+1}|t_it_{i+1})}{\partial t_i} &= \bigg(- iH_S + Lz_{i,t}^* - L^\dagger z_{i+1,t}\\ &\quad -L^\dagger\hat{O}(z_{i+1}z_i^*,t_i,t_{i+1})\bigg) + \mathcal{O}((t_i-\tau)^2),\end{aligned} \tag{2.86}$$

where

$$\begin{aligned}\hat{O}(z_{i+1}z_i^*,t_i,t_{i+1}) &= \int_{t_{i+1}}^{t_i} d\tau\alpha(t_i-\tau)O(z_{i+1}z_i,t_i,\tau) =\\ &= g_0(t_i,t_{i+1})L + g_1(t_i,t_{i+1})\bigg(- i[H_S,L] + g_0(t_i,t_{i+1})[L^\dagger,L]L\bigg)\\ &- z_{i+1,t}g_1(t_i,t_{i+1})[L^\dagger,L].\end{aligned} \tag{2.87}$$

The last expression can be defined in terms of a new operator $\hat{O}'(t_i,t_{i+1})$ as

$$\hat{O}(z_{i+1}z_i^*,t_i,t_{i+1}) = \hat{O}'(t_i,t_{i+1}) - z_{i+1,t}g_1(t_i,t_{i+1})[L^\dagger,L], \tag{2.88}$$

where

$$\hat{O}'(t_i,t_{i+1}) = g_0(t_i,t_{i+1})L + g_1(t_i,t_{i+1})\bigg(- i[H_S,L] + g_0(t_i,t_{i+1})[L^\dagger,L]L\bigg). \tag{2.89}$$

In the last equations we have defined the following set of functions,

$$g_\gamma(t_i,t_{i+1}) = \int_{t_{i+1}}^{t_i} d\tau\alpha(t_i-\tau)(t_i-\tau)^{(\gamma)}, \tag{2.90}$$

for $\gamma = 0, 1, 2$. Arranging together the terms depending on the environmental coordinates z_i and z_{i+1}, we have

$$\begin{aligned} \frac{\partial G(z_i^* z_{i+1}|t_i t_{i+1})}{\partial t_i} &= \bigg(- iH_S + Lz_{i,t}^* - P(t_i, t_{i+1}) z_{i+1,t} \\ &- L^\dagger \hat{O}'(t_i, t_{i+1}) \bigg) + \mathcal{O}((t_i - \tau)^2), \end{aligned} \tag{2.91}$$

where we have defined

$$\begin{aligned} P(t_i, t_{i+1}) &= L^\dagger \Big(1 - g_1(t_i, t_{i+1})[L^\dagger, L] \Big) \hat{O}'(t_i, t_{i+1}) = \\ &= g_0(t_i, t_{i+1}) L + g_1(t_i, t_{i+1}) \Big(- i[H_S, L] + g_0(t_i, t_{i+1})[L^\dagger, L] L \Big). \end{aligned} \tag{2.92}$$

In the particular case of $z_{i+1} = 0$ the previous result of [54] is obtained.

2.4.4 Relation between weak coupling and near Markov approximation

There is a relation between the correlation time τ_c, the weak coupling parameter g, and the maximum time t_m up to which any of the corresponding approximations (namely near Markov and weak coupling respectively) are valid. Thus, when interactions become highly non-Markovian, so τ_c increases, t_m remains constant only if the square of the coupling parameter g decreases at the same rate. This can be seen more clearly with an example. Let us suppose that we have a two level system dipolarly coupled with a Lindblad operator $L = \sigma_{12}$ and a total Hamiltonian given by (2.1). As it will be studied in more detail in Chapter (12), the population of the upper level is in general given by

$$\frac{d\rho_{22}(t)}{dt} = -2g^2 \int_0^t d\tau \Re\{\hat{\alpha}(t-\tau)\} \rho_{22}(\tau) + \mathcal{O}(g^3), \tag{2.93}$$

which up to second order in the perturbative parameter g is

$$\rho_{22}(t) = \rho_{22}(0) \left[1 - 2g^2 \int_0^t dl \int_0^l d\tau \Re[\hat{\alpha}(l-\tau) \right] + \mathcal{O}(g^4). \tag{2.94}$$

The population ρ_{22} should always be $0 < \rho_{22} < 1$, in such a way that, if $\rho_{22}(0) = 1$, then it is necessary that

$$\left[1 - 2g^2 \int_0^t dl \int_0^l d\tau \Re[\hat{\alpha}(l-\tau) \right] < 1. \tag{2.95}$$

The limit condition is then defined as

$$\frac{1}{g^2} = 2 \int_0^{t_m} dl \int_0^l d\tau \Re[\hat{\alpha}(l-\tau)] \tag{2.96}$$

where t_m is the maximum time in which the condition is fulfilled. For a simple exponentially decaying correlation $\alpha(t) = \exp(-\Gamma t)$, the condition reads as follows,

$$t_m = \frac{1}{\tau_c g^2}, \tag{2.97}$$

which illustrates the relation between correlation time and perturbative parameter, and therefore the equivalence between the weak coupling and Markov approximation. A new aspect of this equivalence is discussed in the next chapter, when it is shown that both approximations lead to the same master equation.

2.5 STOCHASTIC INTERPRETATION OF THE REDUCED PROPAGATOR.

As discussed in the first chapter, our knowledge of the system could be such that if the bath frequecies $\omega'_\lambda s$ and the coupling constants $g'_\lambda s$ **are known**. Then, it is possible to construct the functions z_t as

$$z_{i,t} = i \sum_\lambda g_\lambda z_{i,\lambda} e^{-i\omega_\lambda t}, \tag{2.98}$$

and the correlation function $\alpha(t)$ with (2.41). Then, if we were able to perform the integrations over the coherent state variables $z_{i,\lambda}$ according to the measure $d\mu(z_i)$, we would obtain the MTCF following (2.12), and the master equation (2.13). However, the complex Gaussian integrals over coherent states can only be completely done in the very special case of a solvable model (for instance if $L \propto H_S$).

In general, some numerical or approximate schemes are needed.

- A numerical way is to choose at random a set of coherent state coordinates $z = \{z_1, \cdots, z_\lambda, \cdots\}$ that are distributed according to the measure $d\mu(z)$, i.e such that

  $$z_\lambda = \xi_1 + i\xi_2, \tag{2.99}$$

  where ξ_i, with $i = 1, 2$ is a Gaussian distributed real noise. With the set z, and the knowledge of the corresponding coupling strengths g_λ, the functions z_{i,t_i} can be generated from equation (2.41). In that way, we know that the corresponding correlation function $\alpha(t)$, will have the desired form (2.41). Let us emphasize that within this scheme there is no assumption concerning the size of the system or the size of the environment, except those made to go from the equation (2.40) to the equation (2.52). The whole information of the system and environment is available, and we just decide to solve the multidimensional integrals over coherent states by a Monte-Carlo method. As a consequence the better the sampling is, the closer we are to the exact solution of the problem, except for the approximations made, if any, in the equations of motion for the reduced propagators. It turns out that the states of the oscillators that have a mayor contribution are first of all those that are close to the vacuum, (at zero temperature), a fact that is encoded in the measure $d\mu(z)$, and second the pair of coherent states z_i, z_{i+1} that have a significant overlap $\exp(|z_i^* - z_{i+1}|^2)$. This last point is relevant if we want to have a reliable method of stochastic sampling, and it is a consequence of the initial condition for the reduced propagator. If we consider time averages of observables, such overlap is irrelevant but becomes important when computing the MTCF.

- The analytical way is to perform the sum over z through Gaussian multidimensional integrals. In this case it is necessary to use either a weak coupling expansion of the reduced propagators or certain mathematical theorem established by Novikov [104].

Both techniques will be used and discussed in detail in next chapters, both for evolving expectation values or MTCF.

In many applications the detailed information of the environment is **not known**, $i.e$ the individual frequencies $\omega'_\lambda s$ and coupling constants $g'_\lambda s$ are not accessible. At this point we should keep in mind that the only required information of the environment is its correlation function. If $\alpha(t)$ is at our disposal, we can generate a Gaussian distributed set of complex random numbers in such a way that they have the required correlation function (see Appendix (P) and ([35]) for a method). In other words, the synthesis of such complex $noise$ consists in the construction of a bath of oscillators that has the desired correlation function. Once the noise is generated, the equations that rule the dynamics of the system state vectors can be integrated, so that an average over many realizations of the noise leads to the MTCF or to a master equation. Notice that now the environment does not need to be composed of harmonic oscillators. Even though equations (2.40) and (2.52) have been obtained through a microscopical derivation, when $z_{i+1} = 0$ they can be considered as the phenomenological description of the interaction of a system with any environment, provided that the last can be described by a certain fluctuation $z_{i,t}$ with a certain correlation function $\alpha(t)$. The case with $z_{i+1} \neq 0$ is more complicated because the initial condition of $G(z_i^* z_{i+1}|t_i t_{i+1})$ depends on the particular representation used. In the present case, where Bargmann states are used, $G(z_i^* z_{i+1}|t_{i+1} t_{i+1}) = \langle z_i|z_{i+1}\rangle = \exp{(z_i^* z_{i+1})}$.

When the variables z_i and z_{i+1} are chosen randomly, equations (2.40) and (2.52) become SSEs. In addition, when $z_{i+1} = 0$, the second order version of (2.52) coincides with the SSE derived by Diósi, Gisin and Strunz in [40], and later by Strunz in [41].

3

Conclusions of this part

We have presented in this part the general model of Hamiltonian for the systems studied in this thesis, and the general tool we are going to use to this end, namely the reduced propagator.

In Chapter (1), we discuss the Caldeira and Legget Hamiltonian, which describes a system with a single generalized coordinate in contact with a harmonic oscillator environment. Under certain conditions, this system may be reduced to the spin-boson model commonly found in the literature, and which will be studied in Chapter (5) of this thesis. The interaction part of this Hamiltonian describes a linear coupling between an environment and a system operator. A more general Hamiltonian for linear couplings consists in a sum over many environment and system operators. In particular, we show that the Hamiltonian of an atom dipolarly coupled to the radiation field has this form. In the last part of the chapter is introduced the concept of Markovian and non-Markovian interactions. Whether the interaction is Markovian or not is determined by the so-called environmental correlation function. We present such function and discuss some of the different methods used in its generation.

In Chapter (2) we introduce the reduced propagator as a tool to derive many of the dynamical equations used in this thesis. When no approximations are made, the evolution equation of the reduced propagator is an open equation (2.40), belonging to the Hilbert space of the total system. Some approximations can be assumed to reduce it to a closed equation for the reduced propagator into the system Hilbert space, with the general form (2.52). In general, both type of equations depend on two-time dependent functions, z^*_{i,t_i} and z^*_{i+1,t_i}, that take into account the "history" of the environment and lead to a conditioned dynamics of the system with respect to the environment dynamics.

The closed equation (2.52) is used in the Parts (II) and (III) to derive master and MTCF equations up to second order in the perturbative parameter. When $z_{i+1} = 0$, the integration of the equation for the reduced propagator leads to the evaluation of the reduced density operator with initial condition $\rho_s(0) = Tr_S\left(\rho_{tot}(0)\right) = Tr_S\left(|\psi_0\rangle\langle\psi_0| \otimes |0\rangle\langle 0|\right)$, once the average over the final states z_i is performed. For initial environmental state different from the vacuum, $z_{i+1} \neq 0$, the reduced propagator can be used to evaluate multiple time correlation functions, as well as the expectation values of system observables with more general initial conditions.

The open equation (2.40) provides a basic tool to derive in Chapter (III) the hierarchy that MTCF formally obey when no approximations are made.

When the initial and final environmental states are chosen randomly according to their Gaussian distribution, the equation for the reduced propagator, particularly its closed version, may be considered a SSE.

Part II

QUANTUM MEAN VALUES

4

Introduction

In the last chapter we presented the system reduced propagators $G(z_i^* z_{i+1}|t_i t_{i+1})$ as the essential piece to calculate any aspect of the dynamics of a quantum open system, including its expectation values and its fluctuation properties. This chapter examines the former, while the analysis of fluctuations is left for Part (III).

The dynamics of expectation values of operators of a QOS is studied by using master equations that evolve the reduced density matrix $\rho_s(t)$, or SSE that evolve the system wave function [1] $|\psi_t(z^*)\rangle$ in terms of stochastic trajectories. Both schemes are related with each other by

$$\rho_s = \mathcal{M}[|\psi_t(z^*)\rangle\langle\psi_t(z)|] \tag{4.1}$$

where $\mathcal{M}[*]$ denotes the average over the ensemble of trajectories weighted by the distribution of the classical driving noise appearing in the SSE. Depending on the method used in its derivation, there are many different SSE that, having the property (4.1) are called *unravelings* of the reduced density matrix.

In some of these unravelings the stochastic evolution is represented by sudden changes in the wave vector, giving rise to quantum jump trajectories (see for instance [62, 63, 64, 65, 66, 67]). In some others the stochastic increment is a diffusive process and gives rise to the quantum state diffusion model of trajectory (QSD) [68, 69]. This last model has also been extended to non-Markovian interactions [35, 41, 54, 40, 70], and it is the one studied in this thesis. In the last chapter we have already derived non-Markovian SSE from the reduced propagator, where it has also been shown that for a bath of harmonic oscillators, the average appearing in (4.1) is of a Gaussian type $\mathcal{M}[\cdots] \equiv \int d\mu(z)\cdots$ (see equation (2.47)).

In the first part of the chapter we set up the framework for the dynamical equations used in this thesis to describe the evolution of expectation values. A broad description of all the alternative methods that exist in the literature is out of the scope of this work. In consequence, details will only be given when deriving results that are relevant for the present work. The chapter is divided into two parts,

---

[1] By system wave function we mean a vector that lives in the Hilbert space of the system.

- Section (4.1) starts with a brief historical review of Markovian master equations. A more detailed derivation of a non-Markovian master equation within the weak coupling approximation is then discussed. Such equation is later used to describe several systems. We present some references and discuss some alternative non-Markovian master equations.
- Section (4.2) follows the same structure for introducing SSE. Here, the two types of Markovian equation, namely jump-like and diffusive are briefly treated. For non-Markovian interactions some different stochastic schemes are also explained, in order to provide a context for the two particular ones that are studied in this work. The first scheme is the one proposed by Diósi, Strunz and Gisin in [39, 40, 71], which can be derived from the formalism of reduced propagators. The second is the one proposed by Gaspard and Nagaoka in [35]. We note that in the last chapter and in [3, 4], an equation was presented for propagators starting from an arbitrary environmental state, and which can also be interpreted as an stochastic equation.

4.1 MASTER EQUATIONS

4.1.1 Markovian master equation

The theory for describing the dynamics of open quantum system is well developed under the Markov hypothesis, assuming that the relaxation time of the bath is much smaller than any relevant time scale of the system. One of the first evolution equation was derived in 1917 by Einstein [51, 72], and described the atomic population dynamics of an atom emitting and absorbing light in a thermal field. This generalization of this equation, made in 1928 by Pauli [51, 73], reads as follows

$$\begin{aligned}\frac{dP_n(t)}{dt} &= \sum_{m>n}(A^n_m + B^n_m D)P_m(t) + \sum_{m<n} B^n_m D P_m(t)\\ &- \sum_{m<n}(A^m_n + B^m_n D)P_n(t) - \sum_{m>n} B^m_n D P_n(t),\end{aligned} \tag{4.2}$$

where the $P_n(t)$ are the occupation probabilities of the energy levels. The coefficients A^m_n and B^m_n represent the transition rates from the atomic state n to the atomic state m due to spontaneous and stimulated emission respectively. In this equation, $D \equiv D(\omega_{mn})$ is the energy density of the electromagnetic field at the emitting frequency, $\omega_{mn} = (E_m - E_n)$, where E_n is the energy of the level n. The energy density is given by Plank's radiation law, $D(\omega_{mn}) = \alpha\omega^3_{mn} \exp -(\omega_{mn}/\kappa_B T)$ [2].

The positive terms represent the gain of probability from transitions into the state n, and the negative terms represent loss of probability by transitions from the state n. The transition rates between populations $\{A^m_n, B^m_n\}$ are given by the Fermi Golden Rule within the weak coupling approximation [74]. When the Hamiltonian of the system is unknown, transition rates can be calculated from experimental data, or chosen by a phenomenological ansatz. The use of a quantum theory that only has to deal with probabilities was justified by Pauli with the so-called "repeated random phase assumption" [51], which consisted in assuming that the phase relation between wave functions are always (repeatedly) randomized, so that only the square of the wave function (i.e. the probabilities) are relevant.

Later on, a new object was introduced by von-Neumann and Landau [15, 16, 38, 51, 74], the **density operator** $\rho(t)$, which is more convenient to describe systems where the repeated random phase assumption

---

[2] Let us remind here that we have settled $\hbar = 1$, so that $\omega_{mn} = (E_m - E_n)/\hbar \equiv E_m - E_n$ and $D(\omega_{mn}) = \alpha\omega^3_{mn} \exp -(\hbar\omega_{mn}/\kappa_B T) \equiv D(\omega_{mn}) = \alpha\omega^3_{mn} \exp -(\omega_{mn}/\kappa_B T)$.

can not be applied. A good example of those systems are lasers, which were developed in 1960s. A laser is a highly coherent field, so that the Pauli equation is not sufficient to describe either its dynamics or the dynamics of a system interacting with it.

The density operator may in general correspond to a pure quantum state $\rho(t) = |\Psi_t\rangle\langle\Psi_t|$, or to a statistical mixture, $\rho(t) = \sum_k P_k|\Psi_k\rangle\langle\Psi_k|$, where P_k represents the probability of the state $|\Psi_k\rangle$ in the mixture. In general, the density operator of a quantum open system corresponds to the later case. For instance, in Chapter (2) it has been proven that when choosing a coherent state representation for the environment, the reduced density operator is a statistical mixture of vectors $|\psi_t(z^*)\rangle$, where the sum in k is replaced by an integral over the different coherent state eigenvalues $z^* \equiv z_1^* \cdots z_\lambda^* \cdots$. In addition, when the reduced density matrix is represented in the atomic energy basis, the diagonal elements, called populations, correspond to the occupation probabilities P_n computed with the Pauli master equation, while the off-diagonal elements, called coherences, correspond to transitions between the different energy eigenstates of the QOS.

Among the different Markovian master equations proposed in the last decades, the most popular one is the Lindblad equation [36], which gives positive $\rho_s(t)$ for all initial conditions,

$$\frac{d\rho_s(t)}{dt} = -i[H_s, \rho_s(t)] + \frac{1}{2}([L\rho_s(t), L^\dagger] + [L, \rho_s(t)L^\dagger]). \tag{4.3}$$

Although the positivity of the density operator has been considered an important property to be kept by a master equation, it can only be expected for initially decorrelated states between system and environment.

In Appendix (C) it is discussed in detail the problem of positivity of the density operator, as well as its representation in terms of coherences and populations.

4.1.2 Non-Markovian master equations

The first non-Markovian master equation was derived by Redfield within the context of nuclear magnetic resonance [75]. A more precise non-Markovian master equation and the Redfield equation itself was later derived by performing a *second order perturbative approximation* of the von-Neumann equation, which is the evolution equation for the density matrix of the total system [37, 50]. The same equation can also be obtained by making certain considerations about the evolution time scales and using the *Born approximation*, which consists in assuming $\rho_{tot}(t) \approx \rho_s(t) \otimes \rho_B$ [50]. We start this section by deriving the master equation with the Born approximation, and then with the second order perturbative approximation. Furthermore, we show in Appendix (D) that the Born approximation is exact up to second order in the perturbation parameter.

4.1.2.1 Time scales and Born approximation The von-Neumann equation for the density operator of the total system $H_{tot} = H_S + H_B + H_I$ in interaction picture, $\rho_{tot}^I(t)$, reads as follows

$$\frac{d\rho_{tot}^I(t)}{dt} = \frac{1}{i}[V_t H_I, \rho_{tot}^I(t)], \tag{4.4}$$

where $V_t H_I = \mathcal{U}_0^{-1}(t, t_0) H_I \mathcal{U}_0(t, t_0)$, $\rho_{tot}^I = \mathcal{U}_0^{-1}(t, t_0)\rho_{tot}(t)\mathcal{U}_0(t, t_0)$ and the free evolution operator is $\mathcal{U}_0(t, t_0) = \exp[-iH_0(t - t_0)]$. To simplify the notation, we set $\rho_{tot}^I(t) = \rho_{tot}(t)$. We can integrate (4.4) between t_0 and t, with $t - t_0 = \Delta t$. After some iterations and a trace over the bath degrees of freedom, this leads to the following equation,

$$\begin{aligned}\Delta\rho_s(t) &= \frac{1}{i}\int_{t_0}^{t} d\tau Tr_B\{[V_\tau H_I, \rho_{tot}(t_0)]\} \\ &+ \left(\frac{1}{i}\right)^2 \int_{t_0}^{t} d\tau \int_{t_0}^{\tau} d\tau' Tr_B\{[V_\tau H_I, [V_{\tau'} H_I, \rho_{tot}(\tau')]]\},\end{aligned} \tag{4.5}$$

where $\rho_s(t) = Tr_B\{\rho_{tot}(t)\}$ is the system reduced density operator and,

$$\Delta\rho_s(t) = \rho_s(t) - \rho_s(t_0). \tag{4.6}$$

Equation (4.5) is exact, but some assumptions have to be made in order to express it in a more simple way. Choosing the vacuum as the initial environmental state, then $\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0)$, and the average value in $\rho_B(t_0)$ of the coupling $H_I(t)$ is zero,

$$Tr_B[V_{t_0} H_I \rho_B(t_0)] = 0, \tag{4.7}$$

so that the first term in (4.5) can be eliminated. After the change of variable $T = \tau$ and $s = \tau - \tau'$, equation (4.5) becomes,

$$\rho_s(t) = \rho_s(t_0) - \int_{t_0}^{t} dT \int_0^{T-t_0} d\tau Tr_B\{[V_T H_I, [V_{T-\tau} H_I, \rho_{tot}(T-\tau)]]\}. \tag{4.8}$$

The evolution equation for the reduced density operator can be obtained by deriving (4.8) with respect to t,

$$\frac{d\rho_s(t)}{dt} = -\int_0^{t-t_0} d\tau Tr_B\Big([V_t H_I, [V_{t-\tau} H_I, \rho_{tot}(t-\tau)]] \Big), \tag{4.9}$$

with initial condition $\rho_s(t_0)$. In order to transform (4.8) into an equation for ρ_s local in time, it is necessary to perform a *Markovian approximation* over the time evolution of the system. In this approximation, the evolution of ρ_{tot} from t_0 to t is neglected, provided that the domain of integration time $\Delta t = t - t_0$ is small enough in comparison with the evolution time scale of the system T_A ($\Delta t \ll T_A$). Notice that this Markovian approximation, which is related to the evolution time scale of the density operator, is not the same as the Markovian approximation over the bath evolution time scale. In the latter, the correlation time of the bath, τ_c is considered much less than the evolution time of the system ($\tau_c \ll T_A$). In this derivation the Markovian approximation is considered over the density operator, but not over the bath. In that way, the density operator appearing in the right hand side of (4.9) is already local in time, but is still composed of three terms:

$$\rho_{tot}(t) = \rho_s(t) \otimes Tr_S\{\rho_{tot}(t)\} + \rho_{correl}(t). \tag{4.10}$$

The term $\rho_{correl}(t)$, which describes the correlation between the system and the bath at time t, can be neglected with the assumption that $\tau_C \ll \Delta t$, considering that the correlations at time t disappear after a time which is approximately equal to τ_c. This is the so-called Born approximation, which is only valid up to order g^2 in perturbation parameter [50, 76].

With those approximations and choosing $t_0 = 0$, the evolution equation (4.9) becomes,

$$\frac{d\rho_s(t)}{dt} = -\int_0^{t} d\tau Tr_B\{[V_t H_I, [V_{t-\tau} H_I, \rho_B(t) \otimes \rho_s(t)]]\}, \tag{4.11}$$

where $\rho_B(t) = Tr_S\{\rho_{tot}(t)\}$, and the initial condition is $\rho_s(0)$. The two approximations described above are essentially equivalent up to second order in the coupling constant. As discussed in the last chapter, there is a close connection between the relevant time scales of the problem and the coupling parameter between system and environment.

4.1.2.2 Second order perturbative approximation in the coupling constant The equivalence between approximations on time scales and Born approximation, and the weak coupling assumption can be easily seen by returning to (4.4) and performing a perturbative integration of $\rho_{tot}(t)$. After tracing out again the bath's degrees of freedom, we get something very similar to (4.8),

$$\rho_s(t) = \rho_s(t_0) - \int_{t_0}^{t} dT \int_0^T d\tau Tr_B\{[V_T H_I, [V_{T-\tau} H_I, \rho_{tot}(t_0)]]\}, \tag{4.12}$$

but now with $t_0 = 0$ and $\rho_{tot}(t_0)$ instead of $\rho_{tot}(t-\tau)$ inside the integral term. In order to obtain the last expression we have considered the vacuum initial state for the environment, so that $\rho_{tot}(t_0) = \rho_B \otimes \rho_{t_0}$. After deriving equation (4.12) with respect to t, the equation (4.11) is again obtained, once it has been considered that in the second order term, $\rho_s(0)$ can be replaced by $\rho_s(t) + \mathcal{O}(g)$. In summary, the assumptions over the time-scales hierarchy ($\tau_c \ll \Delta t \ll T_A$) are related to the perturbative approximation ($g \ll 1$).

We can replace in (4.11) the general form of H_I given in the first chapter as

$$H_I = \sum_\beta S_\beta B_\beta, \tag{4.13}$$

so that

$$V_t H_I = \sum_\beta V_t \{S_\beta B_\beta\}, \tag{4.14}$$

with

$$\begin{aligned} V_t S_\beta &= \exp(iH_0 t) S_\beta \exp(-iH_0 t) = \exp(iH_S t) S_\beta \exp(-iH_S t), \\ V_t B_\beta &= \exp(iH_0 t) B_\beta \exp(-iH_0 t) = \exp(iH_B t) B_\beta \exp(-iH_B t). \end{aligned} \tag{4.15}$$

In that way, we get

$$\begin{aligned} \frac{d\rho_s(t)}{dt} = -\sum_{\gamma,\beta} \int_0^t d\tau Tr_B([V_t S_\gamma V_t B_\gamma, [V_{t-\tau} S_\beta V_{t-\tau} B_\beta, \rho_s(t) \otimes \rho_B]]) = \\ -\sum_{\gamma,\beta} \Big\{ \int_0^t d\tau (V_t S_\gamma V_{t-\tau} S_\beta \rho_s(t) - V_{t-\tau} S_\beta \rho_s(t) V_t S_\gamma) C_{\gamma\beta}(\tau) \\ + \int_0^t d\tau (\rho_s(t) V_{t-\tau} S_\beta V_t S_\gamma - V_t S_\gamma \rho_s(t) V_{t-\tau} S_\beta) C^*_{\gamma\beta}(\tau) \Big\} \end{aligned} \tag{4.16}$$

where we have defined

$$\begin{aligned} C_{\gamma\beta}(\tau) &= \langle V_t B_\gamma V_{t-\tau} B_\beta \rangle_B \\ C_{\gamma\beta}(-\tau) &= C^*_{\gamma\beta}(\tau) = \langle V_{t-\tau} B_\beta V_t B_\gamma \rangle_B, \end{aligned} \tag{4.17}$$

and we have used the cyclic property of the trace $Tr(ABC) = Tr(CAB) = Tr(BCA)$ to write,

$$\begin{aligned} \langle B_\gamma(t) B_\beta(t-\tau) \rangle_B &= Tr_B(\rho_B B_\gamma(t) B_\beta(t-\tau)) \\ \langle B_\beta(t-\tau) B_\gamma(t) \rangle_B &= Tr_B(\rho_B B_\gamma(t-\tau) B_\beta(t)). \end{aligned} \tag{4.18}$$

The master equation, in interaction image with respect to the system and taking into account the relations between $\{B_\beta\}$, $\{S_\beta\}$ with the Lindblad operator L (equations (1.48) and (1.49) of Chapter (1)), is expressed as [54]

$$\begin{aligned}
\frac{d\rho_s(t)}{dt} &= -i[H_S, \rho_s(t)] + \int_0^t d\tau \alpha^{+*}(t-\tau)[L^\dagger, \rho_s(t)V_{\tau-t}L] \\
&+ \int_0^t d\tau \alpha^{+}(t-\tau)[V_{\tau-t}L^\dagger \rho_s(t), L] \\
&+ \int_0^t d\tau \alpha^{-}(t-\tau)[V_{\tau-t}L \rho_s(t), L^\dagger] \\
&+ \int_0^t d\tau \alpha^{-*}(t-\tau)[L, \rho_s(t)V_{\tau-t}L^\dagger] + \mathcal{O}(g^3),
\end{aligned} \tag{4.19}$$

with

$$\alpha^-(t-\tau) = \sum_\lambda g_\lambda^2 (N(\omega_\lambda)+1) e^{-i\omega_\lambda(t-\tau)}, \tag{4.20}$$

and

$$\alpha^+(t-\tau) = \sum_\lambda g_\lambda^2 N(\omega_\lambda) e^{i\omega_\lambda(t-\tau)}. \tag{4.21}$$

The function $N(\omega) = [\exp(\omega\beta) - 1]^{-1}$,is the average thermal number of quanta in the mode ω. As will be shown in more detail in(5.1.1.2), for the choice (1.48) of $\{B_\beta\}$ the relation between the correlations appearing in the master equation (4.16) and those appearing in (4.19) is $\alpha^\pm(t) = 2\left(C_{11}(t) \pm iC_{21}(t)\right)$ [1].

On the one hand, for zero temperature, $N(\omega)$,$\alpha^+(t-\tau)$ and z^+ are zero, while $\alpha^-(t-\tau)$ becomes equal to

$$\alpha(t-\tau) = \sum_\lambda g_\lambda^2 e^{-i\omega_\lambda(t-\tau)}, \tag{4.22}$$

and the master equation becomes

$$\begin{aligned}
\frac{d\rho_s(t)}{dt} &= -i[H_S, \rho_s(t)] - g^2 \int_0^t d\tau \alpha(\tau) L^\dagger V_{-\tau} L \rho_s(t) \\
&- g^2 \int_0^t d\tau \alpha^*(\tau) \rho_s(t) V_{-\tau} L^\dagger L \\
&+ g^2 \int_0^t d\tau \alpha(\tau) V_{-\tau} L \rho_s(t) L^\dagger \\
&+ g^2 \int_0^t d\tau \alpha^*(\tau) L \rho_s(t) V_{-\tau} L^\dagger.
\end{aligned} \tag{4.23}$$

On the other hand, for $L = L^\dagger = K$, we have

$$\begin{aligned}
\frac{d\rho_s(t)}{dt} &= -i[H_S, \rho_s(t)] - g^2 \int_0^t d\tau \alpha_T(\tau) K V_{-\tau} K \rho_s(t) \\
&- g^2 \int_0^t d\tau \alpha_T^*(\tau) \rho_s(t) V_{-\tau} K K \\
&+ g^2 \int_0^t d\tau \alpha_T(\tau) V_{-\tau} K \rho_s(t) L \\
&+ g^2 \int_0^t d\tau \alpha_T^*(\tau) K \rho_s(t) V_{-\tau} K,
\end{aligned} \tag{4.24}$$

where

$$\alpha_T(t-\tau) = \sum_\lambda g_\lambda^2 \left[\coth\left(\frac{\omega_\lambda \beta}{2}\right) \cos\left(\omega_\lambda(t-\tau)\right) - i \sin\left(\omega_\lambda(t-\tau)\right)\right]. \tag{4.25}$$

The non-Markovian master equation (4.23) leads to the so-called Redfield master equation [75] when $\int_0^t$ can be replaced by $\int_0^\infty$. It is important to point out that the Redfield master equation has been shown to break the positivity of the density matrix for initial conditions near the border of the space of physically admissible density matrices, i.e when $det(\rho_s(0)) \geq 0$ but very close to 0. This issue, which has been a subject of research during the last decade, occurs because the non-Markovian effects that happen at the initial stage of the evolution are not being taken into account when the integral limits of equation (4.23) are extended to infinity [77]. The application of an *slippage* (i.e. a displacement) of initial conditions, first suggested by Suarez and co-workers [78] for the case of a spin-boson model, and then extended by P. Gaspard and M. Nagaoka [37] for general systems, appears to solve this problem.

The non-Markovian memory effects occurring in (4.23) through the integrals over the correlation function $\alpha(\tau)$, may disappear in the Markov approximation, in which $\alpha(\tau) = \delta(\tau)$. In that limit, eq. (4.23) turns out to be the Lindblad master equation (4.3).

Apart from the second order perturbative expansion, there are other methods to derive non-Markovian master equations. The Nakajima-Zwanzing projection operator technique [76, 79, 80] is one of the most well known examples. It is based on a partition of the state of a system into a relevant and an irrelevant part, by defining a suitable projection operator $\mathcal{P}$ which projects the state into the relevant part, and a projector $\mathcal{Q} = 1 - \mathcal{P}$ which projects into the irrelevant part. For a system coupled to an environment, the most common choice of $\mathcal{P}$ is such that

$$\mathcal{P}\rho_{tot}(t) = \rho_s(t) \otimes \rho_B(t), \tag{4.26}$$

where $\rho_s(t) = Tr_B\left(\rho_{tot}(t)\right)$, and therefore there is an effective decorrelation between system and environment. The final equation obtained within this method is quite complicated, since it is an integro-differential equation for $\mathcal{P}\rho_{tot}(t)$, which implies a non-local time dependence on such operator. The so-called time-convolutionless projection operator technique solves this problem, giving rise to an equation for $\mathcal{P}\rho_{tot}(t)$ with a time-local generator $\mathcal{K}(t)$,

$$\frac{d\rho_s(t)}{dt} = \mathcal{K}(t)\rho_s(t) \tag{4.27}$$

which can be derived up to any arbitrary order in the coupling parameter [76]. Specific examples are the time-convolutionless master equation describing spin-relaxation, the spin-boson model, systems coupled to a spin bath, charged particles interacting with an electromagnetic field and the atom-laser (see [81] and references therein). Notice that the second order master equation (4.23) has also the form (4.27).

4.2 STOCHASTIC SCHRÖDINGER EQUATIONS

4.2.1 Markovian SSEs

Stochastic Schrödinger equations were introduced in the 70s within the context of dynamical reduction models [82, 83, 84, 85, 86] (see also [87] for a recent review). In those models (particularly in the so-called Continuous Localization Models) a modified Schrödinger equation is generated which, besides the standard Hamiltonian, contains stochastic terms acting at every time step of the evolution, and nonlinear terms. These new terms induce a diffusion process for the state vector which is responsible for its reduction to a particular subspace or channel in the system's Hilbert space. In Continuous Localization Models the stochasticity is associated to the action of some measurement over the system or some interaction with its environment . For instance, the continuously diffusive non-linear stochastic Schrödinger equation derived by N. Gisin in [83] departs from the von-Neumann-Lüders postulate [15], considering that the stochastic trajectory of the system reduces thanks to a sequence of projective measurements performed by an external apparatus.

In the 90s, N. Gisin and I.C. Percival [88], presented a new SSE very similar to the former one which is driven by a complex white noise, z_t^*, and reads as follows

$$\begin{aligned}\frac{d|\tilde{\psi}_t\rangle}{dt} &= -iH_S|\tilde{\psi}_t\rangle + (L - \langle L\rangle_t)\left(z_t^* + \langle L^\dagger\rangle_t\right)|\tilde{\psi}_t\rangle \\ &\quad -\frac{\Gamma}{2}\left(L^\dagger L - \langle L^\dagger L\rangle\right)|\tilde{\psi}_t\rangle + \mathcal{O}(g^3), \end{aligned} \tag{4.28}$$

in Stratonovich form [51]. The mean value appearing in the former equation is $\langle L^\dagger\rangle = \langle\tilde{\psi}_t|L^\dagger|\tilde{\psi}_t\rangle$, and the complex white noise has the following statistical properties,

$$\begin{aligned}\mathcal{M}[z_t z_\tau^*] &= \Gamma\delta(t-\tau); \\ \mathcal{M}[z_t z_\tau] &= \mathcal{M}[z_t] = 0, \end{aligned} \tag{4.29}$$

where Γ is the dissipative constant and $\mathcal{M}[\cdots]$ denote as usual an average over many realizations of z_t.

In addition, a real valued noise Markovian SSE was presented by G. C. Ghirardi, P. Pearle and A. Rimini [86] also from a dynamical reduction model,

$$\frac{d|\psi_t\rangle}{dt} = -iH_S|\psi_t\rangle + L\xi_t|\psi_t\rangle - \frac{dt\Gamma}{2}L^\dagger L|\psi_t\rangle \tag{4.30}$$

where ξ_t is a real-valued Gaussian white noise such that $\mathcal{M}[\xi_t\xi_\tau] = \alpha(t-\tau) = \Gamma\delta(t-\tau)$ [51, 134]. The former equation is still linear, since it represents the evolution of a non-normalized state. In order to write the density operator as a mixture of pure state vectors, then it has to be transformed into a non-linear equation for normalized states $|\tilde{\psi}_t\rangle$. The transformation is formally made as follows,

$$\frac{d|\tilde{\psi}_t\rangle}{dt} = \frac{d|\psi_t\rangle}{dt}\frac{1}{\sqrt{N}} + |\psi_t\rangle\frac{d}{dt}\frac{1}{\sqrt{N}}, \tag{4.31}$$

where $N = \langle\psi_t|\psi_t\rangle$.

Several models of Markovian SSE have been derived in the frame of theories of continuous observation (see for instance [89, 90, 91, 7]). In those models, contrary to dynamical reduction ones, a particular measuring device is chosen, which determines the kind of trajectory or unraveling that is going to be obtained. In order to minimize the perturbation caused to the system by the measuring device, the measurement is not performed directly on the system but on its environment. Since they are entangled, a measurement of the environment selects the particular state of the mixture compatible with the measurement result. In that way, the quantity that is continuously measured, which is not necessarily the environmental state but a combination of its eigenvalues, is related to the stochastic variable z_t that drives the SSE. Then a sequence of measurement results z_t corresponds to a single trajectory of a Markovian SSE. In other words, the trajectory $|\psi_t(z^*)\rangle$ represents the system state conditioned to the sequence of measurements which have given the result z_t. This kind of measurements that are performed over an auxiliary system (in this case the environment) to which the system of interest is entangled are called *indirect*.

The SSE generated by dynamical reduction models are of **quantum state diffusion** type, since the stochastic element acts on every time step of the trajectory. These diffusive SSE can also be developed in the frame of continuous measurement theories. Particularly, in the frame of quantum optics Carmichael shows that the real noise SSE (4.30) derived by Ghirardi and co-workers in [86] corresponds to continuous homodyne detection [53]. An example of homodyne detection is discussed by P. Goetsch and co-workers in [92] to describe the evolution of an initial Schrödinger cat state of a damped harmonic oscillator. The quantity to be measured in each experimental run is the quadrature of the field emitted by the oscillator $\langle X(t)\rangle_\theta$, where θ is the noise of the trajectory, and the quadrature operator is $X = 1/2(b + b^\dagger)$ (where b and $b^\dagger$ are the annihilation and creation operators of the local oscillator and its phase has been set zero). This output field is put to interfere with a local oscillator of large amplitude and stable phase, in which case sharp values of the noise θ can be measured. In this scheme, which corresponds particularly to a balanced homodyne experiment, the indirect variable to be measured is the continuous noise, and such noise defines a certain diffusive trajectory.

In addition, Wiseman and Milburn showed in [93] that the linear version of the the Gisin and Percival complex noise SSE (4.28), i.e. the equation

$$\frac{d|\psi_t\rangle}{dt} = -iH_S|\psi_t\rangle + Lz_t^*|\psi_t\rangle - \frac{1}{2}L^\dagger L|\psi_t\rangle, \tag{4.32}$$

derived in [89, 90] corresponds to a continuous heterodyne detection of the bath. In the last equation, $z_t^* = \zeta_t = \xi_{1,t} + i\xi_{2,t}$, where $\xi_{i,t}$ with $i = 1, 2$ is a real-valued Gaussian white noise process. The basis chosen for homodyne and heterodyne detection is the quadrature and the coherent basis respectively. A formal derivation of equations (4.30) and (4.32), as well as their correspondence to homodyne and heterodyne detection, is performed by Gambetta and Wiseman in [94] from the measurement theory. This is discussed with some more detail in the next section.

Apart from diffusive trajectories, there exist in the Markovian case quantum trajectories in which the stochastic influence occurs in sudden jumps that interrupt a deterministic non-unitary evolution. The **quantum jumps** formalism was developed first by Zoller, Marte and Walls [62] as a theory to calculate density operators conditioned to different number of photon emissions. The density operator corresponding to the emission of n photons, $\rho_S^{(n)}(t)$, is related with the total density operator by

$$\rho_S^{(n)}(t) = Tr_B\left(P_n\rho_{tot}(t)\right), \tag{4.33}$$

where P_n is the projection operator onto the state of the quantized radiation field that contains n photons. Later on, a formulation of quantum jumps as a stochastic equation was proposed by Hegerfeldt and Wilser [63], Dalibard, Castin and K. Mølmer [65, 66] and Zoller and co-workers [51, 62, 64] (see [67] for more details). In all these methods, a non-Hermitian term and a white noise term is added to the Schrödinger equation. Because of the non-Hermitian term, the trace of the reduced density operator is no longer conserved, being restored again by imposing stochastically chosen quantum jumps. For instance, in the algorithm by Dalibard et. al [65][3], the total wave function at time $t+dt$ is $|\Psi(t+dt)\rangle = |\Psi^{(0)}(t+dt)\rangle + |\Psi^{(1)}(t+dt)\rangle$, where $|\Psi^{(1)}\rangle$ represents the product state of the atom in the ground state $|1\rangle$ and a photon in the field, and $|\Psi^{(0)}\rangle$ represents the product state of an entangled state between atomic ground and excited level and no photon in the field. When a photon is detected, the total state is projected into $|\Psi^{(1)}\rangle$, and when no photon is detected it stays in $|\Psi^{(0)}(t+dt)\rangle$. The probability for a spontaneous emission during dt is given by $dp = \langle\Psi^{(1)}|\Psi^{(1)}\rangle$. The randomness in the detection and no detection of a photon is simulated by numerical generation of a random number ϵ chosen from the interval $[0, 1]$. Thus, when $\epsilon > dp$, it is assumed that no photons are detected, so that $|\Psi(t+dt)\rangle = |\Psi^{(0)}(t+dt)\rangle = \mu(1 - idtH_{eff})$, where $\mu = (1 - dp)^{-1/2}$,

---

[3] Further details of the derivation should be found in the original paper and references therein, but we here give a brief report of the method.

and H_{eff} is a non-Hermitian Hamiltonian. The norm of this state is no longer 1, being given by $1 - dp$. As a consequence, the quantity dp represents the loss of norm of the total state when no photon is detected. When $\epsilon < dp$ a photon is detected and the total state is projected into the normalized state $|\Psi^{(1)}\rangle = |1\rangle \otimes |0\rangle$, where $|1\rangle$ is the atomic ground state (where it is supposed that there had not been time for the atom to be reexcited after having emitted a photon), and the field is reset to the vacuum state (where it has been assumed that the detected photon is destroyed).

As shown in 1993 by Carmichael [53], the Jump-like Markov SSE corresponds to direct photon detection, where the experimental set up consists in a photon counter, and the environmental state is expressed in the number basis. An extended review of the quantum jump approach is found in [67].

Further details of continuous measurement interpretation of Markovian SSE as well as some more references are given in Appendix (E).

4.2.2 Non-Markovian SSE

Several methods have been derived in the last decades to obtain non-Markovian SSE. Some of them are based on *expanding the total wave vector into the environmental basis*. The coefficients of such expansion can be sometimes considered stochastic. In addition, their evolution equation can be computed with the Schrödinger equation for the total wave vector, since they carry all its time dependency. In the last chapter, we have shown that some linear QSD trajectories are obtained within this method by using a Bargmann coherent state basis for the bath. On the one hand, for an initial environmental vacuum state, the following linear equation is obtained up to second order in perturbation parameter g [41]

$$\begin{aligned}\frac{d|\psi_t(z^*)\rangle}{dt} &= -iH_S|\psi_t(z^*)\rangle + Lz_t^*|\psi_t(z^*)\rangle \\ &- L^\dagger \int_0^t d\tau\alpha(t-\tau)V_{\tau-t}L|\psi_t(z^*)\rangle + \mathcal{O}(g^3). \qquad (4.34)\end{aligned}$$

This equation was first derived in 1997 by Diósi, Gisin and Strunz [39]. On the other hand, for a more general initial environmental state z_0, the former equation becomes [3, 4]

$$\begin{aligned}\frac{d|\psi_t(z^*,z_0)\rangle}{dt} &= -iH_S|\psi_t(z^*,z_0)\rangle + Lz_t^*|\psi_t(z^*,z_0)\rangle - L^\dagger z_{0,t}|\psi_t(z^*,z_0)\rangle \\ &- L^\dagger \int_0^t d\tau\alpha(t-\tau)V_{\tau-t}L|\psi_t(z^*,z_0)\rangle + \mathcal{O}(g^3). \qquad (4.35)\end{aligned}$$

In the second part of the chapter both equations, (4.34) and (4.35), are studied in more detail, and we also obtain their non-linear version. Deriving a SSE with this method provides a good way to understand the origin of the stochasticity in the evolution of a quantum open system, as well as the connection between the noise and the particular state of the environment.

Another proposal is the one from Gaspard and Nagaoka [35] who derive a non-Markovian SSE within the so-called *Feshbach projection-operator* method, which is based on the same idea as the Nakajima-Zwanzig projection operator method but is applied to Schrödinger equation ruling the wave function instead of the master equation ruling the density operator. The method is explained in some more detail in the next part of the chapter, where the resulting SSE is also compared to that of Diósi, Gisin and Strunz [1].

A third possibility is to *add fictitious modes* to the non-Markovian system in such a way as to make the enlarged hypothetical system dynamics Markovian again. This method, was first proposed by Imamoglu [95, 96], Garraway [97], and S. Bay and co-workers [98], and then extended by Breuer and co-workers in several works [76, 81]. In the most recent one (see [81] for details), Breuer proposes an enlarged system with density operator W, composed by the original system and a tree level system. The state space of the auxiliary system, C^3, can be spanned by the tree basis states $|a\rangle, |b\rangle, |c\rangle$. The formalization of the method is encoded in the *embedding theorem*, which for that case states that the dynamics of the original system $\rho_s(t)$ can be expressed through the time evolution of a certain set of coherences W_{ab} of the density matrix W of the extended system. The SSE for the wave functions of the extended space $|\Phi_t\rangle$ are Markovian, and therefore have the physical interpretation of continuous measurements. Considering that the extended state space is given by a tensorial product of the original system state space $\mathcal{H}$ and C^3, the states $|\Phi_t\rangle$ can have the general form

$$|\Phi_t\rangle = |\varphi_a(t)\rangle|a\rangle + |\varphi_b(t)\rangle|b\rangle + |\varphi_c(t)\rangle|c\rangle, \tag{4.36}$$

where $|\varphi_k\rangle \,\epsilon\, \mathcal{H}$. Following the embedding theorem we have

$$\rho_s(t) = \frac{\mathcal{M}\left[|\varphi_a(t)\rangle\langle\varphi_b(t)|\right]}{\mathcal{M}\langle\varphi_b(t)|\varphi_a(t)\rangle}. \tag{4.37}$$

Thus, an unraveling is constructed for non-Markovian dynamics which consists in two wave functions, each of them described by a particular Markovian SSE in the extended Hilbert space. The method has some restrictions. First, it starts from the general form of the time-convolutionless equation (4.27), which may not exist for very strong couplings. In addition, the generator of the equation $\mathcal{K}(t)$ is written in terms of certain time-dependent operators belonging to $\mathcal{H}$, to which some restrictions are imposed that might not be valid in certain cases.

Some other methods are based on *continuous measurement* theories. For instance, M.W. Jack, M.J. Collet and D. F. Walls present in [99, 100] a formulation of non-Markovian quantum trajectories which simulate real-time spectral detection of the light emitted from a localized system. In this case, the non-Markovian behavior is not intrinsic to the interaction of the system with its environment, but arises from the uncertainty in the time of emission of particles that are later detected.

In a more recent work, Gambetta and Wiseman propose in [94] a formal way to obtain non-Markovian SSE from a continuous measurement scheme. In their paper they discuss all the mathematical ingredients to describe a continuous measurement [101, 102, 103]. This includes a probability-operator-measure element, or *effect*,

$$\tilde{F}_{\{q_\lambda\}} = |\{q_\lambda\}\rangle\langle\{q_\lambda\}|, \tag{4.38}$$

where $|\{q_\lambda\}\rangle$ is the environmental basis, and $\{q_\lambda\}$ is the result of the measurement. A set of *measurement operators* $\tilde{M}_{q_\lambda}$ is also necessary, with the constraint $\tilde{F}_{\{q_\lambda\}} = \tilde{M}^\dagger_{q_\lambda}\tilde{M}_{q_\lambda}$. For example, we can decompose the measurement operators as

$$\tilde{M}_{q_\lambda} = |\{n_\lambda\}\rangle\langle\{q_\lambda\}|, \tag{4.39}$$

where the final state of the environment after a measurement, $\{n_\lambda\}$ can be chosen as the vacuum, since generally in most detection situations the measurement results in annihilating the detected field. A *noise operator* $\hat{Z}(t)$ is also defined in such a way that

$$\hat{Z}(t)|\{q_\lambda\}\rangle = \hat{z}_t|\{q_\lambda\}\rangle, \tag{4.40}$$

where $\hat{z}_t$ is the noise function from which the conditioned state after a measurement depend. With this definitions at hand, two kind of such conditioned system states after measurement can be obtained. The first state $|\psi_{q_\lambda}(t)\rangle$ is such that: a) depends *linearly* on the premeasurement state $|\psi_t\rangle$, and b) depends on an environmental state $\{q_\lambda\}$ which is distributed according to a probability $\Lambda(\{q_\lambda\})$ that does not take into account the effects of the interaction of the environment, and remains constant in time. In such terms, the linear state after the measurement of $\{q_\lambda\}$ is written as

$$|\psi_{q_\lambda}(t)\rangle = \frac{\langle\{q_\lambda\}|\psi_t\rangle}{\sqrt{\Lambda(\{q_\lambda\})}}. \tag{4.41}$$

Because it is not normalized, the authors argue that the linear conditioned system state does not have a clear physical interpretation, but is useful to derive the actual probability $P(\{q_\lambda\},t)$ that the environmental states have considering its interaction with the system as

$$P(\{q_\lambda\},t) = \langle\psi_{q_\lambda}(t)|\psi_{q_\lambda}(t)\rangle\Lambda(\{q_\lambda\}) \tag{4.42}$$

Such probability is obtained through a Girsanov transformation of the variables $\{q_\lambda\}$ [104]. The Girsanov transformation is explained in some more detail in Appendix H.2. Thanks to this actual probability, it is possible to derive the second kind of conditioned state $|\tilde{\psi}_{q_\lambda}(t)\rangle$ that: a) evolve in a *non-linear* way, and b) depends on an environmental state $\{q_\lambda\}$ that is sampled according to the actual distribution (4.42),

$$|\tilde{\psi}_{q_\lambda}(t)\rangle = \frac{\langle\{q_\lambda\}|\psi_t\rangle}{\sqrt{P(\{q_\lambda\},t)}}. \tag{4.43}$$

A linear SSE can be derived from (4.41) as,

$$\frac{d|\psi_{\{q_\lambda\}}(t)\rangle}{dt} = \frac{\partial|\psi_{\{q_\lambda\}}(t)\rangle}{\partial t} + \sum_\lambda \frac{dq_\lambda}{dt}\frac{\partial|\psi_{\{q_\lambda\}}(t)\rangle}{\partial t}, \tag{4.44}$$

and provided that a Girsanov transformation can be made, a non-linear SSE results in

$$\frac{d|\tilde{\psi}_{\{q_\lambda\}}(t)\rangle}{dt} = \frac{1}{|\psi_{\{q_\lambda\}}(t)|}\frac{d|\psi_{\{q_\lambda\}}(t)\rangle}{dt} + |\psi_{\{q_\lambda\}}(t)\rangle\frac{d}{dt}\frac{1}{|\psi_{\{q_\lambda\}}(t)|}, \tag{4.45}$$

where

$$|\tilde{\psi}_{\{q_\lambda\}}(t)\rangle = \frac{1}{|\psi_{\{q_\lambda\}}(t)|}|\psi_{\{q_\lambda\}}(t)\rangle, \tag{4.46}$$

and $|\psi_{\{q_\lambda\}}(t)| = \langle\psi_{\{q_\lambda\}}(t)|\psi_{\{q_\lambda\}}(t)\rangle$. Since it is normalized, the former state represents, with a probability equal to 1, the conditioned state of the system after a measurement of output $\{q_\lambda\}$ has been performed at time t in the environment. This statement is true no matter whether the interaction is Markovian or non-Markovian. However, the linking of such state with earlier states obtained by evolving (4.45), is only possible in the first type of interaction. Once a measurement of the environmental state has been made at time t, a future measure performed at time $t+\Delta t$ is altered if $\Delta t < \tau_c$. In other words, the measurement at time $t+\Delta t$ is performed before the environment have recovered from the last measurement, since the recovering time is of order τ_c. Considering that $\Delta t \to 0$ for a continuous measurement, only in the Markovian case in which the correlation time $\tau_c = 0$ the sequence of measurements that monitorize a trajectory do not affect each others.

When the environmental basis is chosen as the coherent state basis, $|\{q_\lambda\}\rangle \equiv ||\{z_\lambda\}\rangle$, where $||z_\lambda\rangle$ is a coherent state (see Appendix (B)), the noise operator is

$$\hat{Z}(t) = \sum_\lambda g_\lambda a_\lambda e^{-i\Omega_\lambda t}, \tag{4.47}$$

and therefore the noise function is

$$\hat{z}_t = \sum_\lambda g_\lambda z_\lambda e^{-i\Omega_\lambda t}, \tag{4.48}$$

where $\Omega_\lambda = \omega_\lambda - \omega_S$. The phase factor $i\omega_S t$, appears because the equations derived in the paper are in the interaction picture with respect to the diagonal part of the system Hamiltonian, $H_S = -\omega_S\sigma_z/2$. Except for this factor and a constant i, the last equation corresponds to the noise appearing in the Markov equation (4.32) and in the non-Markovian equation (4.34), obtained by Diósi, Gisin and Strunz [40]. Moreover, the linear equation (4.44) of a coherent unraveling equals the linear equations (4.32) and (4.34) in the Markov and non-Markovian case respectively. The distribution used for the linear equation is the Gaussian

$$\Lambda(\{q_\lambda\}) = \langle 0|z\rangle\langle z|0\rangle = \prod_\lambda \frac{e^{-|z_\lambda|^2}}{\pi}. \tag{4.49}$$

A different unraveling is obtained when choosing a quadrature basis, $|\{q_\lambda\}\rangle \equiv |\{X_\lambda^+, Y_\lambda^-\}\rangle$, with $\{X_\lambda^+\}$ and $\{Y_\lambda^-\}$ the eigenvalues corresponding to the two-mode quadrature operators

$$\begin{aligned} \hat{X}_\lambda^+ &= \frac{\hat{x}_\lambda + \hat{x}_{-\lambda}}{\sqrt{2}} \\ \hat{X}_\lambda^- &= \frac{\hat{y}_\lambda - \hat{y}_{-\lambda}}{\sqrt{2}}, \end{aligned} \tag{4.50}$$

and $\hat{x}_\lambda$, $\hat{y}_\lambda$ the quadratures of the annihilation operator $\hat{a}_\lambda$,

$$\hat{a}_\lambda = \frac{\hat{x}_\lambda + i\hat{y}_\lambda}{\sqrt{2}}, \tag{4.51}$$

the resulting linear equation is a real-valued noise equation. For Markovian interactions, such equation becomes equal to (4.30), and $\hat{z}_t = \sqrt{\Gamma}\xi_t$ is a real-valued Gaussian white noise. For the non-Markovian case, the linear equation is

$$\frac{d|\psi_t(\hat{z})\rangle}{dt} = \left\{-iH_S + \hat{z}_t L - L_X \int_0^t d\tau \beta(t-\tau)\frac{\delta}{\delta\hat{z}_\tau}\right\}|\psi_t(\hat{z})\rangle, \tag{4.52}$$

with $L_X = L + L^\dagger$, which is equal to the linear equation derived by Bassi and Ghirardi in [87] from a dynamical reduction model. In this unraveling, the noise operator is

$$\hat{Z}(t) = \sum_{\lambda>0} 2g_\lambda \left[\hat{X}_\lambda^+ \cos(\Omega_\lambda)t + \hat{Y}_\lambda^- \sin(\Omega_\lambda t)\right], \tag{4.53}$$

and the noise function

$$\hat{z}_t = \sum_{\lambda>0} 2g_\lambda \left[X_\lambda^+ \cos(\Omega_\lambda)t + Y_\lambda^- \sin(\Omega_\lambda t)\right], \tag{4.54}$$

in such a way that

$$\begin{aligned} \mathcal{M}[\hat{z}_t\hat{z}_\tau] &= \beta(t-\tau); \\ \mathcal{M}[\hat{z}_t] &= 0, \end{aligned} \tag{4.55}$$

with $\beta(t-\tau)$ the memory function for the noise,

$$\beta(t-\tau) = 2\sum_{\lambda} g_{\lambda}^{2}\cos\left(\Omega_{\lambda}(t-\tau)\right). \tag{4.56}$$

Hence, for non-Markovian interactions, $\hat{z}_t$ is a real-valued Gaussian coloured noise. The quadrature unraveling corresponds to a very special type of interaction Hamiltonian in which for each mode λ there exists another mode that we can label as $-\lambda$ in such a way that $\omega_{-\lambda} = -\omega_{\lambda}$, and $g_{-\lambda} = g_{\lambda}^{*}$. Thus, the interaction Hamiltonian^4 is

$$H_I = \sum_{\lambda>0} g_{\lambda}\left\{L\left(a_{\lambda}^{\dagger}e^{i\Omega_{\lambda}t} + a_{-\lambda}^{\dagger}e^{-i\Omega_{\lambda}t}\right) - L^{\dagger}\left(a_{\lambda}^{\dagger}e^{-i\Omega_{\lambda}t} + a_{-\lambda}e^{i\Omega_{\lambda}t}\right)\right\}. \tag{4.57}$$

This Hamiltonian could be used as a starting point to derive a SSE by expanding $|\Psi_t\rangle$ in the quadrature basis. It would be interesting to verify if the resulting equation is equal to (4.52). At the end of the chapter, we display in serveral tables the different stochastic equations that exist and the different methods that have been used to derive them. Indeed, the SSE with complex noise (and as noted above maybe also those with real noise, by using (4.57)) can be derived by representing the total wave function $|\Psi_t\rangle$ within a certain environmental basis. To this end, it is important that the coefficients of the expansion can be considered as the stochastic wave vectors^5. The average of all these SSEs correspond to closed master equations for the reduced density matrix. As discussed above, there are several methods for obtaining such closed master equations, but they mostly rely in assuming some approximation, like the weak coupling or the near-Markov approximations ^{6}. As an example, the time-convolutionless projection operator technique (TCL) consists in a systematic perturbative expansion for the time-dependent generator of the master equation (4.27). However, for strong couplings such an expansion becomes very complicated, so that obtaining a master equation is not feasible in practice. In order to avoid the problems of a perturbative expansion, Breuer propose in [60, 61] a method which is based on reconstructing the total density matrix as the expectation value of a pair of stochastic vectors $|\Phi_1(t)\rangle, |\Phi_2(t)\rangle$, such that

$$\rho_{tot} = \mathcal{M}[|\Phi_1(t)\rangle\langle\Phi_2(t)|], \tag{4.58}$$

where $\mathcal{M}$ denotes a certain stochastic average. It is supposed that the stochastic state vectors are direct product states of certain system states $\psi_\nu \in \mathcal{H}_S$, and environmental states $\xi_\nu \in \mathcal{H}_B$, where $\mathcal{H}_S$ and $\mathcal{H}_B$ are the system and environmental Hilbert space respectively. Notice that the total density matrix is not decomposed into the environmental basis. Thus,

$$|\Phi_\nu(t)\rangle = \psi_\nu(t)\otimes\xi_\nu(t);\ \nu = 1, 2, \tag{4.59}$$

---

[4] Expressed in interaction image with respect to the environment and H_S.

[5] This can be seen easily when a coherent state basis is chosen for the environment, since in this basis the measure $d\mu(z)$ is a Gaussian function. Nevertheless, for a general basis some assumptions have to be made. For instance, the Feshbach projection-operator method used in [35] to derive a SSE decomposes the total wave vector in a general (discrete) environmental basis. In this derivation, the stochastic interpretation comes from the assumption that the environment is composed of a large number of harmonic oscillators, and moreover, that the equivalent classical system is chaotic. Thus, the quantities appearing in the evolution of the system wave vector which are sum over environmental eigenvalues, can be considered as noises through the central limit theorem. This is explained in more detail in the original paper [35] and in Appendix (F) of this thesis.

[6] For instance, in Chapter (2) we have seen that the evolution equation of the coefficients of the expansion of $|\Psi_t\rangle$ in a coherent state basis, namely $G(z_i^* z_{i+1}|t_i t_{i+1})|\psi_0\rangle$, is *open*, i.e. it does not only depend on the coefficient that is being evolved, but on a set of them. In order to obtain a *closed* equation which can be interpreted as a SSE, it is in general necessary to perform some of the approximation described in the same chapter.

and

$$\rho_s(t) = Tr_B(\rho_{tot}) = \mathcal{M}[|\psi_1(t)\rangle\langle\psi_2(t)|\langle\xi_2(t)|\xi_1(t)\rangle]. \tag{4.60}$$

The stochastic differential equations for the $\psi_\nu(t)$ and the $\xi_\nu(t)$ are then constructed in such a way that $|\Phi_\nu(t)\rangle$ reproduces the exact von-Neumann equation with (4.58). These equations have the structure of quantum jumps, with a term that represents the periods of deterministic evolution (drift terms), and a term that provide the contribution from random instantaneous jumps. The method have two mayor advantages: it gives the exact solution of the von-Neumann equation, and it is valid for other couplings as well as the linear ones on which most of the former SSE are based. Furthermore, it provides the possibility of determining numerically MTCF even in the non-Markovian case. Nevertheless, first, to our knowledge there is not an analytic way to perform the averages $\mathcal{M}[\cdots]$, so that no explicit equation of non-Markovian MTCF can be obtained, and second, when the environmental degrees of freedom is large, the number of spinorial components of the vector $\xi_\nu(t)$ is also large, what might make the numerical convergence slower. For instance, the electromagnetic field is described through a continuous set of harmonic oscillators, that would give rise in principle to environmental vectors of infinite dimension.

DYNAMICAL REDUCTION

H_I	z_t	$\alpha(t-\tau)$	**Equation**
No model	Real White	$\mathcal{M}[\hat{z}_t\hat{z}_\tau] = \Gamma\delta(t-\tau)$	Eq. (4.30)
No model	Real Coloured	$\mathcal{M}[\hat{z}_t\hat{z}_\tau] = \Re\alpha(t-\tau)$	Eq. (4.52)
No model	Complex White	$M[z_t z_\tau^*] = \Gamma\delta(t-\tau)$	Eq. (4.32)

MEASUREMENT

H_I	z_t	$\alpha(t-\tau)$	**Equation**
$H_I = \sum_{\lambda>0} g_\lambda\{L\left(a_\lambda^\dagger e^{i\omega_\lambda t} + a_{-\lambda}^\dagger e^{-i\omega_\lambda t}\right)$ $-L^\dagger\left(a_\lambda^\dagger e^{-i\omega_\lambda t} + a_{-\lambda} e^{i\omega_\lambda t}\right)\}$	Real white: $\hat{z}_t = \sqrt{\Gamma}\xi_t$	$\mathcal{M}[\hat{z}_t\hat{z}_\tau] = \Gamma\delta(t-\tau)$	Eq. (4.30)
Idem	Real coloured: $\hat{z}_t = \sum_{\lambda>0} 2g_\lambda\{X_\lambda^+ \cos(\omega_\lambda)t$ $+Y_\lambda^- \sin(\omega_\lambda t)\}$	$\mathcal{M}[\hat{z}_t\hat{z}_\tau] = \Re\alpha(t-\tau)$	Eq. (4.52)
$H_I = \sum_\lambda g_\lambda\left\{a_\lambda^\dagger L + L^\dagger a_\lambda\right\}$	Complex white: $\hat{z}_t = \sqrt{\Gamma}\zeta_t = \sqrt{\Gamma}(\xi_{1,t} + i\xi_{2,t})$	$M[z_t z_\tau^*] = \Gamma\delta(t-\tau)$	Eq. (4.32)
Idem	Complex coloured: $\hat{z}_t = -iz_t$	$\mathcal{M}[z_t z_\tau^*] = \alpha(t-\tau)$	Eq. (4.34)

EXPANSION $|\Psi_t\rangle$

H_I	z_t	$\alpha(t-\tau)$	**Equation**
$H_I = \sum_\lambda g_\lambda\left\{a_\lambda^\dagger L + L^\dagger a_\lambda\right\}$	Complex white: $z_t = -i\sum_\lambda g_\lambda z_\lambda e^{-i\omega_\lambda t}$	$M[z_t z_\tau^*] = \Gamma\delta(t-\tau)$	Eq. (4.32)
Idem	Complex coloured: $z_t = -i\sum_\lambda g_\lambda z_\lambda e^{-i\omega_\lambda t}$	$\mathcal{M}[z_t z_\tau^*] = \alpha(t-\tau)$	Eqs. (4.34) and (4.35)

5

Quantum mean values a non-Markovian QOS

In the last chapter we have discussed the different derivations of SSEs that appear in literature, both Markovian and non-Markovian, as well as the interpretation that the first type of equations have in terms of continuous measurement. In this chapter, we intend to particularize to the non-Markovian SSE derived from the Feshbach projection operator method, and from reduced propagators when they are considered as stochastic objects. In addition, as introduced in Chapter (2), if reduced propagators are not considered stochastic, they can be used to derive master equations for all the different situations that can be encountered, provided that a closed equation of $G(z_i^*, z_{i+1}|t_i t_{i+1})$ can be found, and that the analytical average over the z_i^* and z_{i+1} can be made. The situations here treated are summarized as follows,

- The system and the environment are initially decorrelated, so that

  $$\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0). \tag{5.1}$$

  We consider two cases: ρ_B corresponding to the vacuum state $\rho_B = |0\rangle\langle 0|$ (although it can also be written as a thermal reservoir at zero temperature), and ρ_B a thermal state. In both cases ρ_B can be expressed in the coherent state P representation as $\rho_B = \int d\mu(z_0)P(z_0^*, z_0)|z_0\rangle\langle z_0|$.

  For such initial conditions,

  $$\rho_s(t) = \int d\mu(z) \int d\mu(z_0) P(z_0^* z_0) G(z^* z_0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^* z|0t), \tag{5.2}$$

  $$\langle A\rangle = Tr_S(\rho_s(t)A), \tag{5.3}$$

- The system and the environment are initially correlated, so that

  $$\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0) + \rho_{correl}(t_0), \tag{5.4}$$

where the last term ρ_{correl} denotes a certain initial correlation. For instance, this situation corresponds to

$$|\Psi_0\rangle = \int d\mu(z_0)|\psi_0(z_0^*)\rangle|z_0\rangle \tag{5.5}$$

so that the reduced density matrix becomes

$$\rho_s(t) = \int d\mu(z_0) \int d\mu(z_0')\rho_s(z_0 z_0'^*|t), \tag{5.6}$$

where we have defined

$$\rho_s(z_0 z_0'^*|t) = \int d\mu(z_1)G(z_1^* z_0|t0)\rangle|\psi_0(z_0^*)\rangle\langle\psi_0(z_0')|G^\dagger(z_0'^* z_1|t0). \tag{5.7}$$

The motivation of this chapter is double folded: First, we study and compare some of the different SSE in the literature, in order to prove their correspondence to the master equation, as well as their efficiency in terms of number of trajectories needed to obtain ρ_s. Second, we use the reduced propagators to derive some master equations corresponding to some of the different initial conditions above described. According to this, the chapter is then divided in two sections:

- In Section (5.1), we focus in the evaluation of quantum mean values by performing a numerical *sampling of different stochastic trajectories*. Although there is no continuous measurement interpretation for non-Markovian SSE, their usefulness is not only related to their interpretation in terms of trajectories of the state vector of a measured system. Without making any attempt to give a physical meaning to single stochastic trajectories, the SSEs are useful to compute the quantum mean values of a QOS, being sometimes more efficient than master equations. Such efficiency of the SSE with respect to master equations depends on two factors: 1) that the system degrees of freedom is large, and 2) that the sampling of the SSE is good, so that a small number of trajectories is needed to perform the averages. The first factor is intrinsic to the problem under study, whereas the second depends on the particular SSE that is chosen. In the first section we try to answer the question of which are the SSE that improve the sampling, or, to be more exact, when such improvement is significant enough. It is argued that temperature of the environment is an important parameter to take into account, and we show this in Section (5.1.3) for a spin boson system.

- In Section (5.2), we show how reduced propagators can be used to *derive master equations* by performing analytically the average over different trajectories. In addition, thanks to the reduced propagator, a master equation is derived which is more general than the existing ones, since it allows the evolution of system density operators which are initially entangled with the environment, as well as a master equation for non-zero temperature.

As usual, the coupling parameter g, is defined as $g[H_0] = [H_I]$, where $H_0 = H_S + H_B$. The model Hamiltonian chosen is the same as in Chapter (2),

$$\begin{aligned} H &= H_S + H_B + H_I \\ &= H_S + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda + \sum_\lambda g_\lambda \left(a_\lambda^\dagger L + L^\dagger a_\lambda\right). \end{aligned} \tag{5.8}$$

5.1 STUDY OF THE SAMPLING OF STOCHASTIC SCRÖDINGER EQUATIONS

As noted in the introduction, the stochastic Schrödinger equation scheme may provide a significant numerical advantage over the master equation approach, in particular, as soon as the Hilbert space dimension $\mathcal{F}$ of the QOS is large. In order to obtain ρ_s, the stochastic approach only needs to integrate a state of dimension $\mathcal{F}$ for a certain number of realizations κ. In contrast, the solution of the master equation demands the integration of $\mathcal{F}^2/2$ elements of the density operator. If the number of realizations of the stochastic scheme is not too large (which also depends on the accuracy one aims to achieve), then stochastic Schrödinger equations may be in practice more advantageous than master equations, being intrinsically paralelizable. A more accurate comparison of the performance of both methods can be found in [38], where the time needed to numerically compute the quantum mean value of a certain operator is studied both with the master equation (T_{ME}) and with the stochastic sampling (T_{SSE}), the latter one within a certain standard error. The relation between both times is such that

$$\frac{T_{ME}}{T_{SSE}} \propto \mathcal{F}^{1+x}, \tag{5.9}$$

where x is a parameter that depends on the operator, but generally is equal to 0 or 1. Evidently, the former is a rough relation. In a more precise calculus, the time T_{SSE} is found to be dependent on the number of realizations of the stochastic process (also number of trajectories κ) that are necessary to reproduce the result with a certain accuracy. Therefore, to be numerically efficient it may be very important to choose a stochastic equation giving solutions with a significant weight in the average

$$\rho_s(t) = \frac{\mathcal{M}[|\psi_t(z^*)\rangle\langle\psi_t(z)|]}{\mathcal{M}[\langle\psi_t(z)|\psi_t(z^*)\rangle]}, \tag{5.10}$$

so that the number of trajectories needed κ in the stochastic scheme is small. In other words, it is important to choose the SSE that provides the best possible sampling. Although $\mathcal{M}[\langle\psi_t(z)|\psi_t(z^*)\rangle] = \mathrm{Tr}\,(\rho_s(t)) = 1$, in practical applications along the chapter the use of (5.10) leads to more stable results, since such average of the norm is performed numerically and might have not converged to one. As we have seen in Chapter (2), the distribution of states of the bath, $\exp(-|z|^2) = \exp(\sum_\lambda z_\lambda^* z_\lambda)$ also corresponds to that of the variable z_t, since it is composed with the sum $z_t = i\sum_\lambda z_\lambda g_\lambda \exp(-i\omega_\lambda t)$. Therefore, in the equation of the reduced propagator, once the variable z_t is considered as a noise, it is sampled over the same Gaussian distribution during the whole evolution. The equation of the vacuum reduced propagator, that is *linear* with the wave function, gives rise to two different equations within the weak coupling limit, a *convoluted* equation in which the evolution of $|\psi_t(z^*)\rangle$ is local in time, and a *non-convoluted* equation in which it is not. These two linear equations, which corresponds to environments at zero temperature, are studied in detail in Section (5.1.1.1), where it is also shown that they are equivalent with each other up to second order in the perturbation parameter. The extension of each equation to a model valid at environmental temperatures different from zero is made in Section (5.1.1.2). In such section, two different derivations are described, the one performed in [41, 39, 54, 40, 71], and the one presented in [35].

In certain situations the system-environment interaction is responsible for a significant displacement of the environment oscillators from their initial values. This means that if we keep on sampling the oscillator eigenvalues according to a Gaussian distribution centered at the origin, they will give stochastic solutions with negligible weight in the sum (5.10). In other words, since the interaction is also affecting the bath, a Gaussian distribution centered at the origin might become a poor description of its statistics. To overcome this problem, a second kind of stochastic Schrödinger equation has been proposed, in which the noise probability distribution is considered in evolution during the interaction [41, 40]. Due to such dynamical dependence in its statistics, the equation appears to have a more complicated form than any of the linear ones, showing a *non-linear* dependence with the wave function. Non-linear equations are more convenient especially in situations where the environmental oscillators, and in consequence their probability distribution (which is also the one corresponding to the noise), is considerably altered during the interaction. In particular, this situation occurs in the high temperature regime, in which the non-linear equation has been shown to present a much more efficient sampling than the linear ones [6]. This result, exemplified with the spin-boson model, will be further explained in Section (5.1.3).

5.1.1 Non-Markovian *linear equation*: convoluted and convolutionless

In the non-Markovian regime there are several suitable types of Stochastic equations. In some of these equations, the noise probability distribution is not considered in evolution during the interaction with the system, resting as a Gaussian centered at the origin at all times. These are linear equations. Depending on the derivation and assumptions made, two different linear equations appear in literature: a linear equation derived in [39, 71, 54, 41] which is local in time for the wave function (here referred as *non-convoluted* equation), and a second time non-local equation derived by Gaspard and Nagaoka [35], referred here as the *convoluted* equation. Although different in form, both equations are equivalent up to order g^2 in the coupling constant [1]. We study in the first place two linear equations suitable for environments at zero temperature and weak couplings. The extension of those equations to non-zero temperatures is obtained in Section (5.1.1.2), where new models of correlation function appear due to the temperature dependence.

5.1.1.1 Zero temperature. Two linear stochastic equations, convoluted and non-convoluted, are presented in this section. The evolution equation (2.40) for the reduced propagator $G(z_i^* z_{i+1}|t_i t_{i+1})$, can be used to derive a SSE. For a total system with initial state $|\Psi_0\rangle = |\psi_0\rangle|0\rangle$, we have $|\psi_t(z^*)\rangle = G(z^*0|t0)|\psi_0\rangle$, where we have eliminated the subindex i, and made $z_{i+1} = 0$ and $t_{i+1} = 0$. We then have the following SSE,

$$\begin{aligned}\frac{d}{dt}|\psi_t(z^*)\rangle &= -iH_S|\psi_t\rangle + gLz_t^*|\psi_t(z^*)\rangle \\ &- g^2L^\dagger\int_0^t d\tau\alpha(t-\tau)\frac{\delta|\psi_t(z^*)\rangle}{\delta z_\tau^*},\end{aligned} \tag{5.11}$$

where the quantity $\frac{\delta|\psi_t(z^*)\rangle}{\delta z_\tau^*}$ is a functional derivative of $|\psi_t(z^*)\rangle$ with respect to z_t^*. This equation, as well as the vacuum reduced propagator $G(z^*0|t0)$, was first derived by W. T. Strunz and Diósi in [39, 41]. As derived in Chapter (2), the variable z_t is the following combination of coherent state labels z_λ,

$$z_t^* = -i\sum_\lambda g_\lambda z_\lambda^* e^{iw_\lambda t}, \tag{5.12}$$

where ω_λ represents the frequency of the λ oscillator. Changing to interaction picture with respect to the subsystem, the equation (5.11) becomes:

$$\frac{d}{dt}|\psi_t^I(z^*)\rangle = gV_tLz_t^*|\psi_t^I(z^*)\rangle - g^2V_tL^\dagger\int_0^t d\tau\alpha(t-\tau)\frac{\delta|\psi_t^I(z^*)\rangle}{\delta z_\tau^*}, \tag{5.13}$$

where as usual $V_tL = e^{iH_St}Le^{-iH_St}$ and $|\psi_t(z^*)\rangle = e^{iH_St}|\psi_t^{sp}(z^*)\rangle$, and the index I represents the interaction picture. Equation (5.11) (or its interaction picture version (5.13)), is equal to the equation (2.45) for the propagator with $z_{i+1} = t_{i+1} = 0$, and once the propagator is applied to $|\psi_0\rangle$. As explained in [41] and Section (2.5), they are just a particular representation of the Schrödinger equation for the system and the environment, representing an evolution in the total system state space. The equations only become stochastic when, for practical reasons we have to choose random realizations of the variables z_λ appearing in z_t^* to perform the sum (5.10), establishing a sort of Montecarlo method that permits to consider z_t^* as a noise. The statistical properties of z_t are such that:

$$\begin{aligned} \mathcal{M}[z_t] = 0, \mathcal{M}[z_t z_\tau] = 0 \\ \mathcal{M}[z_t z_\tau^*] = \alpha(t-\tau), \end{aligned} \tag{5.14}$$

where $\alpha(t-\tau)$ is the correlation function of z_t, the *noise*, defined in (2.42) as in (4.22).

Once we consider z_t^* as an stochastic variable, the two terms of (5.13) can be interpreted as follows: the first one represents a stochastic forcing against the system produced by the fluctuations of the bath, and the last term represents the damping or dissipation, also caused by the interaction with the bath. Whether a convoluted or a non-convoluted stochastic equation is obtained from (5.13) depends on the treatment of the functional derivative $\frac{\delta|\psi_t\rangle(z^*)}{\delta z_\tau^*}$. In particular, as described in Chapter (2), the following form is proposed as an ansatz in [54, 40, 71],

$$\frac{\delta|\psi_t(z^*)\rangle}{\delta z_\tau^*} = O(t,\tau,z_t)|\psi_t(z^*)\rangle, \tag{5.15}$$

where $O(t,\tau,z_t)$ is a linear operator that has to be constructed for each case. Notice that replacing (5.15) into equation (5.13) we obtain a non-convoluted equation, as the time dependence of the wave function remains local during the evolution. Naturally, such equation is equal to the closed equation (2.52) for a vacuum propagator once the last one is applied to an initial state $|\psi_0\rangle$.

Within the weak coupling approximation scheme developed in chapter (2) (a result obtained in [41, 55] for the case of a vacuum propagator), the operator $O(t,\tau,z_t)$ is, up to zero order

$$O(t,\tau,z) = V_{\tau-t}L + \mathcal{O}(g). \tag{5.16}$$

It should be stressed that since the noise term is of order g, and the dissipative term is at least of order g^2 (due to the presence of the correlation function of the noise), only such zero term is necessary for a second order linear stochastic equation. With (5.16), the second order non-convoluted linear equation becomes:

$$\frac{d}{dt}|\psi_t(z^*)\rangle = gV_tLz_t^*|\psi_t(z^*)\rangle - g^2V_tL^\dagger\int_0^t d\tau\alpha(t-\tau)V_\tau L|\psi_t(z^*)\rangle. \tag{5.17}$$

A convoluted linear stochastic equation, analogous to the one obtained in [35], can now be deduced by performing a perturbative integration of equation (5.13),

$$\begin{aligned} |\psi_t(z^*)\rangle - |\psi_0\rangle &= g\int_0^t d\tau z_\tau^* V_\tau L|\psi_0\rangle \\ &+ g^2\int_0^t d\tau V_\tau L z_\tau^* \int_0^\tau d\tau' z_{\tau'}^* V_{\tau'} L|\psi_0\rangle \\ &- g^2\int_0^t d\tau V_\tau L^\dagger \int_0^\tau d\tau'\alpha(\tau-\tau')V_{\tau'}L|\psi_0\rangle + \mathcal{O}(g^3), \end{aligned} \tag{5.18}$$

and then applying the functional derivative $\frac{\delta|\psi_t(z^*)\rangle}{\delta z_\tau^*}$. Since the functional derivative already appears in a second order term in g, we restrict ourselves to terms of order g^0, so that

$$\frac{\delta|\psi_t(z^*)\rangle}{\delta z_\tau^*} = V_\tau L|\psi_\tau(z^*)\rangle + \mathcal{O}(g). \tag{5.19}$$

Here, following a perturbative integration of the wave function, similar to (5.18) but from 0 to τ, we have settled that $|\psi_0\rangle = |\psi_\tau(z^*)\rangle + \mathcal{O}(g)$, up to the zero order needed. Notice that the non-convoluted equation can also be obtained with this method, by considering that, at the same order, it is also true that $|\psi_0\rangle = |\psi_t(z^*)\rangle + \mathcal{O}(g)$. Let us here point out that in order to keep the correct dependence on the perturbative variable, it should be taken into account that the functional derivative with respect to z^*_τ is in fact equivalent to $\frac{\delta(*)}{\delta(g z^*_\tau)}$. Finally, the linear convoluted equation obtained substituting (5.19) in (5.13) is

$$\frac{d}{dt}|\psi_t(z^*)\rangle = gV_t L z^*_t |\psi_t(z^*)\rangle - g^2 V_t L^\dagger \int_0^t d\tau \alpha(t-\tau) V_\tau L |\psi_\tau(z^*)\rangle. \tag{5.20}$$

5.1.1.2 Non-zero temperature So far, the stochastic equation was derived for an initial state at zero temperature, corresponding to $|\Psi_0\rangle = |\psi_0\rangle|0\rangle$ for the total state. A more general linear stochastic Schrödinger equation, valid for baths at finite temperature, can be derived by canonically mapping the nonzero temperature density operator of the heat bath onto the zero-temperature density operator of a larger hypothetical environment [40]. The resulting finite temperature linear equation is

$$\begin{aligned}\frac{d}{dt}|\psi_t\rangle &= -iH_S|\psi_t\rangle + gLz^-_t|\psi_t\rangle + gL^\dagger z^+_t|\psi_t\rangle \\ &- g^2 L^\dagger \int_0^t \alpha^-(t-\tau)\frac{\delta|\psi_t\rangle}{\delta z^-_\tau}d\tau \\ &- g^2 L \int_0^t \alpha^+(t-\tau)\frac{\delta|\psi_t\rangle}{\delta z^+_\tau}d\tau. \end{aligned}\tag{5.21}$$

For simplicity we have dropped the explicit dependence of the wave function on the two independent Gaussian noises z^-_t and z^+_t, which have zero means and the following correlations:

$$\begin{aligned}\mathcal{M}[z^-_t z^-_\tau] &= 0, \\ \mathcal{M}[z^{-*}_t z^-_\tau] &= \alpha^-(t-\tau) = \sum_\lambda g^2_\lambda (N(\omega_\lambda)+1)e^{-i\omega_\lambda(t-\tau)}, \\ \mathcal{M}[z^+_t z^+_\tau] &= 0, \\ \mathcal{M}[z^{+*}_t z^+_\tau] &= \alpha^+(t-\tau) = \sum_\lambda g^2_\lambda N(\omega_\lambda)e^{i\omega_\lambda(t-\tau)} \\ \mathcal{M}[z^{+*}_t z^-_\tau] &= 0. \end{aligned}\tag{5.22}$$

Again one can try to replace the functional derivatives in (5.21) by an ansatz of type (5.15). Using a perturbative expansion for $O(t,\tau,z)$ we again find

$$\begin{aligned}\frac{\delta|\psi_t\rangle}{\delta z^-_\tau} &= O^-(t,\tau,z^\pm)|\psi_t\rangle = V_{\tau-t}L|\psi_t(z^*)\rangle + \mathcal{O}(g), \\ \frac{\delta|\psi_t\rangle}{\delta z^+_\tau} &= O^+(t,\tau,z^\pm)|\psi_t\rangle = V_{\tau-t}L^\dagger|\psi_t\rangle + \mathcal{O}(g). \end{aligned}\tag{5.23}$$

It can be easily checked that the ensemble average of (5.21) leads to the master equation (4.19). Notice that at zero temperature, the linear stochastic equation (5.13) is re-obtained, since for this case $N(\omega)$, $\alpha^+(t-\tau)$ and z^+ are zero, while $\alpha^-(t-\tau)$ becomes equal to (4.22). For finite temperature and a Hermitian coupling operator $L = L^\dagger = K$ equation (5.21) is simplified as

$$\frac{d}{dt}|\psi_t\rangle = -iH_S|\psi_t\rangle + gKz_t|\psi_t\rangle$$

$$-g^2 K \int_0^t d\tau \alpha_T(t-\tau) V_{\tau-t} K|\psi_t\rangle + \mathcal{O}(g^3). \tag{5.24}$$

where now the noise is $z_t = z_t^+ + z_t^-$ and has the following statistical properties:

$$\begin{aligned} \mathcal{M}[z_t z_\tau] &= 0, \\ \mathcal{M}[z_t^* z_\tau] &= \alpha^-(t-\tau) + \alpha^+(t-\tau) = \alpha_T(t-\tau) \\ &= \sum_\lambda g_\lambda^2 \left[\coth\left(\frac{\omega_\lambda \beta}{2}\right) \cos\left(\omega_\lambda(t-\tau)\right) - i\sin\left(\omega_\lambda(t-\tau)\right)\right], \end{aligned} \tag{5.25}$$

this latter being the standard bath correlation function at non-zero temperature [20, 105], previously defined in (4.25). Clearly, as the temperature goes to zero, $\alpha_T(t-\tau)$ coincides with the zero-temperature expression (4.22).

A second linear non-Markovian stochastic Schrödinger equation has been proposed by Gaspard and Nagaoka [35]. In this section it will be shown that their equation is equivalent to (5.21) up to the relevant second order in the coupling parameter g, although its derivation is based on very different hypothesis. Following [35], let us start from a general Hamiltonian for a system and its environment in the form

$$H_{tot} = H_S + H_B + H_I = H_0 + gV, \tag{5.26}$$

with $H_0 = H_S + H_B$ and an interaction potential V that we assume takes the form

$$V = V^\dagger = \sum_\beta S_\beta B_\beta. \tag{5.27}$$

The Hermitian subsystem and bath coupling operators are S_β and B_β, respectively. This form of the interaction Hamiltonian covers our earlier model (5.8) by choosing two contribution $\beta = 1, 2$ in the sum, with

$$S_1 = L + L^\dagger \, ; \, S_2 = i(L - L^\dagger), \tag{5.28}$$

and

$$B_1 = \frac{1}{2}\sum_\lambda g_\lambda (a_\lambda + a_\lambda^\dagger) \, ; \, B_2 = \frac{i}{2}\sum_\lambda g_\lambda (a_\lambda - a_\lambda^\dagger). \tag{5.29}$$

In this approach to a stochastic equation the total wave function is again expanded, here in the basis of eigenfunctions of the bath $\{|n\rangle\}$, to get

$$|\Psi_t\rangle = \sum_n |\psi_t^n\rangle |n\rangle. \tag{5.30}$$

As before, the ensemble of system states $|\psi_t^n\rangle$ recovers the mixed reduced density operator. The evolution of each of these states will depend on the evolution of others through a set of coupled differential equations. Due to this mutual interaction, and provided that the number of system states is sufficiently large, they will behave in a random way. This brings the idea of deriving a stochastic Schrödinger equation, which evolves only one member of the ensemble of system states $|\psi_t^n\rangle$, under the assumption that such a state is statistically representative of the rest. To decouple the evolution equation of such a state from the time evolution of the rest, the Feshbach projection-operator method is used. Using a perturbative expansion in the coupling strength, and for the special choice of operators (5.28) and (5.29), the following equation is obtained,

$$\frac{d}{dt}|\psi_t\rangle = -iH_S|\psi_t\rangle + g\left(L\eta_A(t) + L^\dagger \eta_B(t)\right)|\psi_t\rangle$$

$$
\begin{aligned}
&- 2g^2 L^\dagger \int_0^t d\tau \, [C_{11}(\tau) - iC_{21}(\tau)] \, V_{-\tau} L e^{-iH_S\tau} |\psi_{t-\tau}\rangle \\
&- 2g^2 L \int_0^t d\tau \, [C_{11}(\tau) + iC_{21}(\tau)] \, V_{-\tau} L^\dagger e^{-iH_S\tau} |\psi_{t-\tau}\rangle + \mathcal{O}(g^3),
\end{aligned}
\tag{5.31}
$$

where the selected system state $|\psi_t^l\rangle$ now represents the wave function $|\psi_t(\eta_A, \eta_B)\rangle \equiv |\psi_t\rangle$. The variables $\eta_A(t)$ and $\eta_B(t)$ are the combinations,

$$
\begin{aligned}
\eta_A(t) &= \eta_2(t) - i\eta_1(t) \\
\eta_B(t) &= -\eta_2(t) - i\eta_1(t),
\end{aligned}
\tag{5.32}
$$

with

$$
\eta_i(t) \equiv \sum_{m(\neq l)} \langle l|V_t B_i|m\rangle e^{-\beta(\epsilon_m - \epsilon_l)/2} e^{i(\theta_m - \theta_l)}. \tag{5.33}
$$

It is assumed that the $\{\theta_i\}$ form a set of independent random phases, uniformly distributed in the interval $[0, 2\pi]$, and ϵ_m and ϵ_l are eigenvalues corresponding to eigenfunctions $|m\rangle$ and $|l\rangle$ of the bath Hamiltonian, respectively. The stochastic nature of equation (5.31) is contained in the behavior of $\eta_i(t)$. If the number of states is large enough to perform the sum (5.33) over a large set of phases $\{\theta_m\}$, these quantities can be characterized as Gaussian random variables by the central limit theorem. As complex Gaussian variables, $\eta_i(t)$ satisfy the following statistical properties,

$$
\begin{aligned}
\mathcal{M}\left[\eta_i(t)\right] &= 0\,;\, \mathcal{M}\left[\eta_i(t)\eta_j(\tau)\right] = 0 \\
\mathcal{M}\left[\eta_i(t)\eta_j^*(\tau)\right] &= C_{ij}^*(t-\tau).
\end{aligned}
\tag{5.34}
$$

Following the definition (5.33) for the noise and since $\mathcal{M}[\exp\left(i(\theta_m - \theta_n)\right)] = \delta_{mn}$, the noise correlation is given by,

$$
\mathcal{M}\left[\eta_i(t)\eta_j^*(\tau)\right] = \sum_n e^{\beta(\epsilon_l - \epsilon_n)} \langle l|V_t B_i|n\rangle\langle n|V_\tau B_j|l\rangle, \tag{5.35}
$$

or equivalently,

$$
\mathcal{M}\left[\eta_i(t)\eta_j^*(\tau)\right]\big|_l = \frac{Z_b}{e^{-\beta\epsilon_l}} \langle l|V_t B_i \rho_b^{eq} V_\tau B_j|l\rangle, \tag{5.36}
$$

where $\rho_b^{eq} = Z_b^{-1}\exp(-H_b\beta)$ is the bath density matrix in equilibrium. In order to obtain the typical value of this correlation function, a thermal average is performed (see [35] and references therein for further details), so that

$$
\sum_l \frac{e^{-\beta\epsilon_l}}{Z_b} \, \mathcal{M}\left[\eta_i(t)\eta_j^*(\tau)\right]\big|_l = \mathrm{Tr}_b[\rho_b^{eq} V_\tau B_j V_t B_i] = C_{ij}^*(t-\tau). \tag{5.37}
$$

With the choice (5.29) for the bath coupling operators B_1 and B_2 we find

$$
\begin{aligned}
C_{12}(t) &= -C_{21}(t) = \frac{i}{4}\sum_\lambda g_\lambda^2 \left\{N(\omega_\lambda)e^{i\omega_\lambda t} - \left(N(\omega_\lambda)+1\right)e^{-i\omega_\lambda t}\right\} \\
C_{11}(t) &= C_{22}(t) = \frac{1}{4}\sum_\lambda g_\lambda^2 \left\{N(\omega_\lambda)e^{i\omega_\lambda t} + \left(N(\omega_\lambda)+1\right)e^{-i\omega_\lambda t}\right\},
\end{aligned}
\tag{5.38}
$$

where the thermal averages of $a_\lambda, a_\lambda^\dagger$ are [51],

$$
\begin{aligned}
\mathrm{Tr}_b\left[\rho_b^{eq} a_\lambda(0) a_\lambda(0)\right] &= 0, \\
\mathrm{Tr}_b\left[\rho_b^{eq} a_\lambda^\dagger(0) a_{\lambda'}(0)\right] &= \delta_{\lambda\lambda'} N(\omega_\lambda),
\end{aligned}
\tag{5.39}
$$

and $N(\omega_\lambda)$ is again the average thermal number of quanta in the mode ω_λ. With expressions (5.39), the combinations $2\left(C_{11}(t) \pm iC_{21}(t)\right)$ appearing in equation (5.31) are equal to the correlation functions $\alpha^{\pm}(t)$ of (5.22), as it was already noted in Section (4.1.2), and the noise combinations η_A and η_B are equal respectively to the noises z^- and z^+ of that equation. As in the previous approach, when we consider the case of a system coupling operator L that is Hermitian $L = L^\dagger = K$, we find

$$\begin{aligned} \frac{d}{dt}|\psi_t(z^*)\rangle &= -iH_S|\psi_t(z^*)\rangle + gKz_t|\psi_t(z^*)\rangle \\ &- g^2K\int_0^t d\tau\alpha_T(t-\tau)V_{\tau-t}Ke^{-iH_S(t-\tau)}|\psi_\tau(z^*)\rangle + \mathcal{O}(g^3), \end{aligned} \tag{5.40}$$

where we have already changed the notation for the noise, $\eta_B(t) + \eta_A(t) \equiv z_t$.

Let us now show how equation (5.24) derived in [41, 39] and equation (5.40) obtained in [35] are equivalent up to order g^2. Indeed, it is consistent with the second order approximation to substitute the wave function $|\psi_\tau(z^*)\rangle$ appearing in the dissipative term of equation(5.40) by its expansion up to order g^0 only. For that it is enough to see that $|\psi_\tau(z^*)\rangle = \left(e^{-iH_S\tau} + \mathcal{O}(g)\right)|\psi_0\rangle$ and furthermore, $|\psi_0\rangle = \left(e^{iH_St} + \mathcal{O}(g)\right)|\psi_t(z^*)\rangle$. Replacing this expression for $|\psi_0\rangle$ in the expression for $|\psi_\tau(z^*)\rangle$, we conclude that

$$|\psi_\tau(z^*)\rangle = \left(e^{iH_S(t-\tau)} + \mathcal{O}(g)\right)|\psi_t(z^*)\rangle. \tag{5.41}$$

Therefore, within second order in the coupling strength g, equation (5.40) becomes equal to the convolutionless equation (5.24). The same holds true for its non-Hermitian version (5.31), which becomes equal to equation (5.21). Clearly, this equivalence also extends to the zero temperature equations.

5.1.2 Non-Markovian *non-linear equations*

As noted in [40], the *linear equation* has an important drawback. During the evolution of the trajectories, which is driven by an input noise governed by the initial state of the bath, the solutions $|\psi_t(z^*)\rangle$ may lose their norm and therefore statistical relevance. This problem comes from not having considered that the interaction between the system and the bath not only affects the system, but also the bath itself. To see this more clearly (see [41] for further details) let us define the Husimi function (or Q-function) of the bath as

$$Q_t(z,z^*) = \frac{e^{-|z|^2}}{\pi}\langle z|\mathrm{Tr}_s\left[|\Psi_t\rangle\langle\Psi_t|\right]|z\rangle, \tag{5.42}$$

where $|z\rangle$ denotes a coherent state of the bath in the Bargmann basis. Since each of these states corresponds to a certain value of the noise the function $Q_t(z,z^*)$ may be interpreted as the probability distribution of the noise. The substitution of $|\psi_t(z^*)\rangle = \int d\mu(z)|\psi_t(z^*)\rangle\langle\psi_t(z)| \otimes |z\rangle\langle z|$ in (5.42) gives the following expression,

$$Q_t(z,z^*) = \langle\psi_t(z)|\psi_t(z^*)\rangle Q_0(z,z^*), \tag{5.43}$$

with $Q_0(z,z^*)$ the initial Gaussian distribution of coherent states $Q_0(z,z^*) = \frac{e^{-|z|^2}}{\pi}$. In terms of (5.43), the density operator (5.10) can be defined as a mixture of pure normalized states weighted by $Q_t(z,z^*)$,

$$\rho_t = \int d^2z\, Q_t(z,z^*)\frac{|\psi_t(z^*)\rangle\langle\psi_t(z)|}{\langle\psi_t(z)|\psi_t(z^*)\rangle}. \tag{5.44}$$

With this expression it is clearer to see that, once the interaction is “switched on” and the environmental oscillators start to move away from the origin according to the distribution $Q_t(z,z^*)$, the states

$$|\psi_t(z^*)/\langle\psi_t(z)|\psi_t(z^*)\rangle^{1/2}, \tag{5.45}$$

which according to $Q_0(z, z^*)$ correspond to small z, will have a decreasing weight in the sum (5.44).

The Husimi function shows a closed time evolution of Liouville form for the set of oscillators z_λ composing the quantity z_t, corresponding to the following phase space flow (see [40] and Appendices (5.46) and (H) for further details of the derivation):

$$\dot{z}_\lambda^* = ig_\lambda e^{-i\omega_\lambda t}\langle L^\dagger\rangle_t. \tag{5.46}$$

In terms of the trajectories $z(t)$ that follow this flow, the Husimi function $Q_t(z, z^*)$ at time t can be expressed as

$$Q_t(z, z^*) = \int d^2 z_0\, Q_0(z_0, z_0^*)\delta^2(z - z(t)), \tag{5.47}$$

where somewhat symbolically, $z(t)$ represents the set of solutions of the different trajectories of the oscillators starting from the set of initial values $\{z_\lambda^*(0) = z_{\lambda,0}^*\}$. In that way, we can now replace (5.44) by an integral of wave functions evaluated in the dynamical states $z^*(t) \equiv \{z_\lambda^*(t)\}$ as

$$\begin{aligned}\rho_t = \int d^2 z_0\, Q_0(z_0, z_0^*)\frac{|\psi_t(z^*(t))\rangle\langle\psi_t(z^*(t))|}{\langle\psi_t(z^*(t))|\psi_t(z^*(t))\rangle} = \\ \int \frac{d^2 z_0}{\pi} e^{-|z_0|^2}\frac{|\psi_t(z^*(t))\rangle\langle\psi_t(z^*(t))|}{\langle\psi_t(z^*(t))|\psi_t(z^*(t))\rangle}.\end{aligned} \tag{5.48}$$

Now, to perform the integral (5.48) with a Monte-Carlo method, a new stochastic variable $\tilde{z}_t^*$ is defined, which corresponds to $z^*(t)$ with a random selection of the initial values for the environmental oscillators $\{z_\lambda^*(0)\}$. From the flow equation (5.46), one obtains

$$\tilde{z}_t^* = z_t^* + g\int d\tau \alpha^*(t-\tau)\langle L^\dagger\rangle_\tau. \tag{5.49}$$

Here, the variable z_t^* is the noise as it appears in the linear stochastic Schrödinger equation, which corresponds to the stationary statistics with distribution function $Q_0(z, z^*)$. The last term represents a dynamical shift or displacement of each z_t which depends on the history of the interaction with the system. The stochastic equation for the wave function $|\psi(z(t))\rangle$ with a shifted noise in the driving term is [40]

$$\begin{aligned}\frac{|\psi_t(z^*(t))\rangle}{dt} &= -iH_S|\psi_t(z^*(t))\rangle + gL\tilde{z}_t^*|\psi_t(z^*(t))\rangle \\ &- g^2(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t, z^*(t))|\psi_t(z^*(t))\rangle,\end{aligned} \tag{5.50}$$

with $\bar{O} = \int_0^t d\tau\alpha(t-\tau)O(t,\tau,z^*(t))$. In order to make clear that the wave function now depends on the shifted noise, we show this dependency explicitly through the notation $|\psi_t(z^*(t))\rangle$. By evolving (5.50) we ensure that the wave functions $|\psi_t(z^*(t))\rangle$ correspond to those realizations that contribute with a significant probability (importance sampling), which according to (5.49) is ensured by the shift term. It is important to note that the difference between the original and the shifted noise is of order of the coupling strength parameter g. Thus, the contribution of the shift turns out to be of the relevant order g^2 in the evolution of the wave functions.

We see from (5.48) that the reduced density operator can now be written as a mixture of normalized stochastic states,

$$\rho_t = \int \frac{d^2 z_0}{\pi} e^{-|z_0|^2}|\tilde{\psi}_t(z^*(t))\rangle\langle\tilde{\psi}_t(z^*(t))| \tag{5.51}$$

with $|\tilde{\psi}_t(z^*(t))\rangle = |\psi_t((z^*(t)))\rangle/\sqrt{\langle\psi_t((z^*(t))|\psi_t(z^*(t))\rangle}$. From (5.50) one obtains an evolution equation for these normalized states [40], giving

$$\frac{d|\tilde{\psi}_t(z^*(t))\rangle}{dt} = -iH_S|\tilde{\psi}_t(z^*(t))\rangle + g(L - \langle L^\dagger\rangle)\tilde{z}_t^*|\tilde{\psi}_t(z^*(t))\rangle$$

$$- \quad g^2[(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,\tilde{z}_t) - \langle(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,z^*(t))\rangle]|\tilde{\psi}_t(z^*(t))\rangle \qquad (5.52)$$

Let us now investigate the three equations described above, the *linear* (5.13), the *shifted* (5.50) and the *non-linear* (5.52) equation by applying them to a spin-boson model. We are interested in studying the numerical equivalence of both linear equations that has been already proved analytically. Finally, we will focus on the problem of sampling, and the convenience of using a linear or a non-linear stochastic Schrödinger equation.

5.1.3 Importance of temperature in the sampling: The spin-boson model

A spin-boson model consists of a two-level system (or a spin $s = \frac{1}{2}$) coupled to a thermal bath of bosonic harmonic oscillators. Defining the Pauli matrices σ_z and σ_x as usual,

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

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

the spin-boson model takes the form of the total Hamiltonian (5.8),

$$H_{tot} = -\frac{\Delta}{2}\sigma_z + g\sum_\lambda g_\lambda \sigma_x(a_\lambda + a_\lambda^\dagger) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda, \qquad (5.53)$$

where Δ is the energy splitting between the two levels, g is the coupling parameter, and σ_x is the coupling operator of the system with the bath. Here we have chosen $\Delta = 0.1$ and $g = 0.1$. Since in this model $L = \sigma_x = L^\dagger$, we use the master equation (4.24), the linear equation (5.24) (equal to (5.21) for $L = L^\dagger = K$), the *shifted* equation (5.50), and the *non-linear* equation (5.52). In addition, they are all computed using the correlation function given by (5.25), which can be expressed as follows in terms of the spectral function $J(\omega)$

$$\alpha_T(t) = \int_0^\infty d\omega J(\omega)\left[\coth\left(\frac{\omega\beta}{2}\right)\cos(\omega t) - i\sin(\omega t)\right]. \qquad (5.54)$$

Here, $J(\omega)$ is the spectral strength,

$$J(\omega) = \frac{\omega^3}{\omega_c^2}\exp(-\omega/\omega_c), \qquad (5.55)$$

where ω_c is a cutoff frequency [35], here chosen as $\omega_c = 1$.

5.1.3.1 Comparison of the linear equations

The linear equation (5.24), which reads as follows for the present case,

$$\frac{\partial|\psi_1(t)\rangle}{dt} = -iH_S|\psi_1(t)\rangle + z_t^*|\psi_2(t)\rangle - \int_0^t d\tau\alpha(t-\tau)e^{-i\Delta(\tau-t)}|\psi_1(t)\rangle$$
$$\frac{\partial|\psi_2(t)\rangle}{dt} = iH_S|\psi_2(t)\rangle + z_t^*|\psi_1(t)\rangle - \int_0^t d\tau\alpha(t-\tau)e^{i\Delta(\tau-t)}|\psi_2(t)\rangle, \qquad (5.56)$$

where $|\psi_t(z)\rangle = \{|\psi_1(t)\rangle, |\psi_2(t)\rangle\}$. The convoluted linear equation (5.31), for $L = L^\dagger$ is equivalent to the former equation but replacing $|\psi_i(t)\rangle$ by $|\psi_i(t-\tau)\rangle$ for $i = 1, 2$ in the integrals. It has been shown at the end

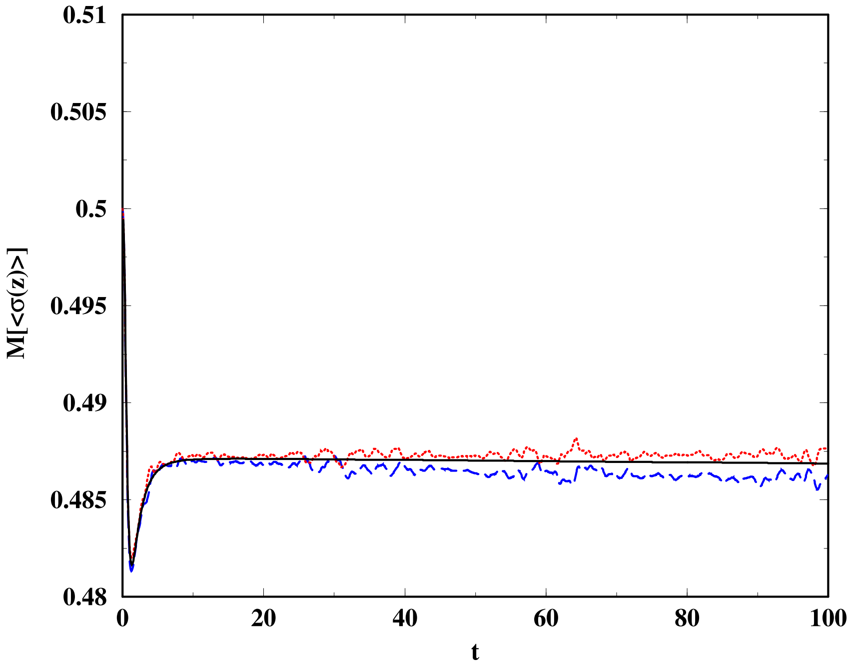

Fig. 5.1 Comparison of the convolutionless linear equation (5.24) (dotted line) and the convoluted linear equation (5.40) (long dashed line) for the same number of trajectories ($\kappa = 10000$). It can be observed that both equations present the same degree of approximation to the non-Markovian master equation (4.24) (solid line). The difference between them increases with time as the second order approximation becomes less accurate.

of Section (5.1.1.2) that the linear equation (5.21) with the perturbative replacement (5.23) of the functional derivative is equivalent to (5.31) up to second order in g. Figure 5.1 confirms this expectation where we compare the ensemble averaged result of both equations obtained with the same number of trajectories, with that of the master equation. Indeed, the difference between each result and the master equation is approximately equal, and the discrepancy between both results increases with time as the effects of the perturbation becomes more important and the second order approximation less accurate.

5.1.3.2 Norm of the wave function We first study the norm of the *linear equation* (5.13) and the *shifted equation* (5.50) for a single trajectory representative of the rest. As we see in Fig. 5.2, norm preservation is lost after very few time steps for high temperatures. In the lower temperature case (Fig. 5.3), the norm of the solutions of either equation is clearly more stable than for the high temperature $\beta = 0.01$, and remains approximately bounded in the time interval studied. Finally, the non-linear normalized equation (5.52) properly maintains the norm provided that the time step of the numerical integration of the equations is small enough to avoid the problems derived from its discretization. In practice, one keeps the states properly normalized numerically.

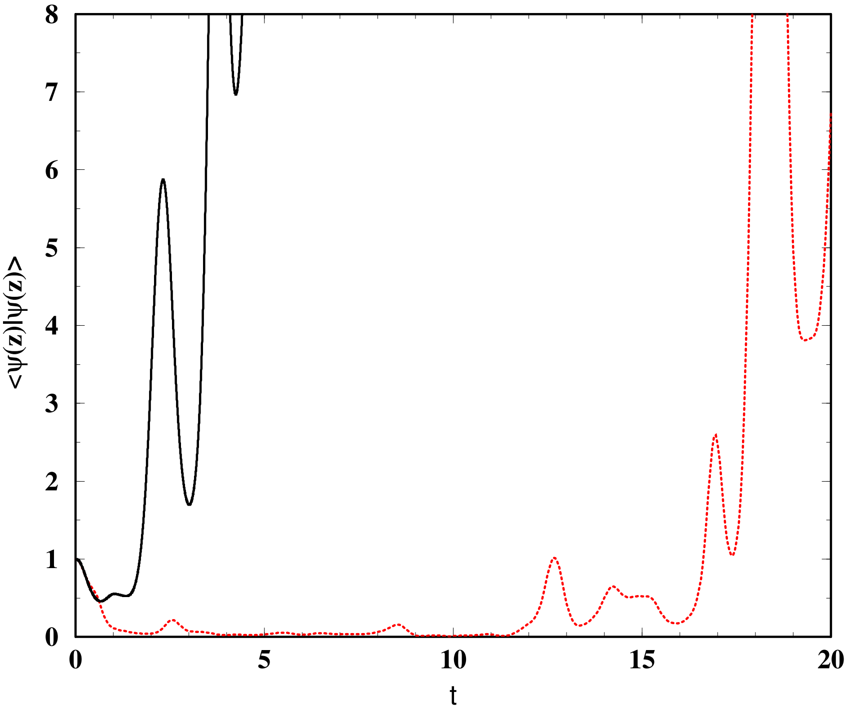

Fig. 5.2 Evolution of the norm of a single trajectory for high temperature, $\beta = 0.01$ using the *linear equation* (5.13) (dotted line), and the *shifted equation* (5.50) (solid line).

5.1.3.3 Ensemble averaged results at different temperatures We have seen in the last section that norm preservation is rapidly lost at high temperatures. However, the important aspect is that despite of this problem, the *shifted equation* (5.50) gives good averaged results. Averaging with the same number of trajectories, the linear equation, in contrast, presents a solution which during the evolution becomes more and more fluctuating and far away from the master equation curve. For this model, the shifted equation has the form

$$
\begin{aligned}
\frac{\partial|\psi_1(z^*(t))\rangle}{dt} &= -iH_S|\psi_1(z^*(t))\rangle + \tilde{z}_t^* \left[|\psi_2(z^*(t))\rangle - \langle\sigma_x\rangle|\psi_1(z^*(t))\rangle\right] \\
&- \int_0^t d\tau\alpha(t-\tau)\left[e^{-i\Delta(\tau-t)}|\psi_1(z^*(t))\rangle + \langle\sigma_x\rangle e^{i\Delta(\tau-t)}|\psi_2(z^*(t))\rangle\right]
\end{aligned}
\tag{5.57}
$$

$$
\frac{\partial|\psi_2(z^*(t))\rangle}{dt} = iH_S|\psi_2(z^*(t))\rangle + \tilde{z}_t^* \left[|\psi_1(z^*(t))\rangle - \langle\sigma_x\rangle|\psi_2(z^*(t))\rangle\right]
$$

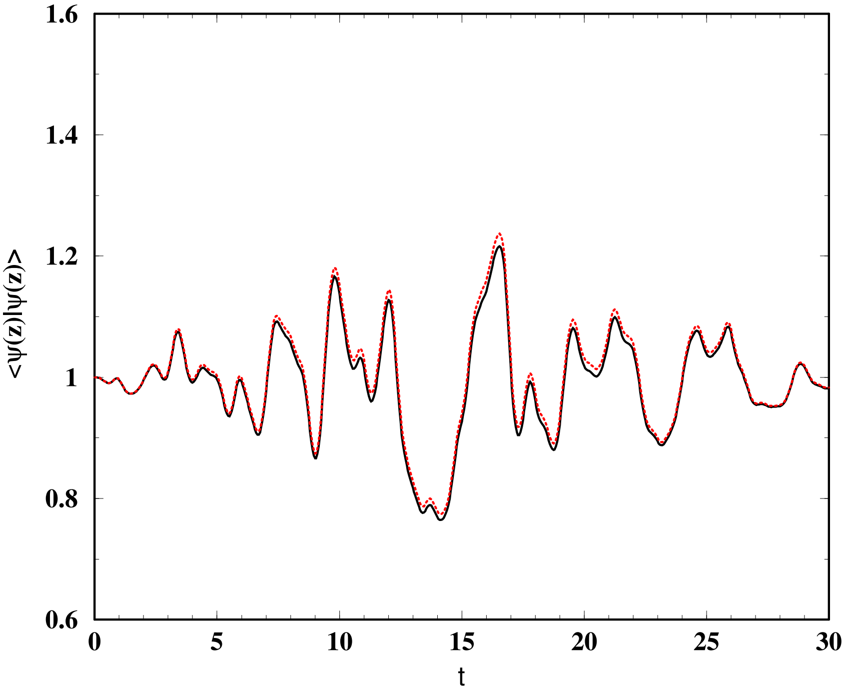

Fig. 5.3 Same as Fig. 5.3 but for low temperature, $\beta = 10$.

$$- \int_0^t d\tau \alpha(t-\tau) \left[e^{i\Delta(\tau-t)} |\psi_2(z^*(t))\rangle + \langle \sigma_x \rangle e^{-i\Delta(\tau-t)} |\psi_1(z^*(t))\rangle \right], \tag{5.58}$$

where $\tilde{z}_t^* = z_t^* + \int_0^t d\tau \alpha(t-\tau) \langle \sigma_x \rangle$, and $\langle \sigma_x \rangle = \langle \psi(z_t) | \sigma_z | \psi(z_t) \rangle / \langle \psi(z_t) | \psi(z_t) \rangle$. These results, shown in Figs. 5.4 and 5.5 for $\kappa = 100$ and $\kappa = 10000$ trajectories respectively, suggest that the shift becomes essential for the true evolution at high temperature, improving significantly the results in comparison with those of the *linear* (non-shifted) equation.

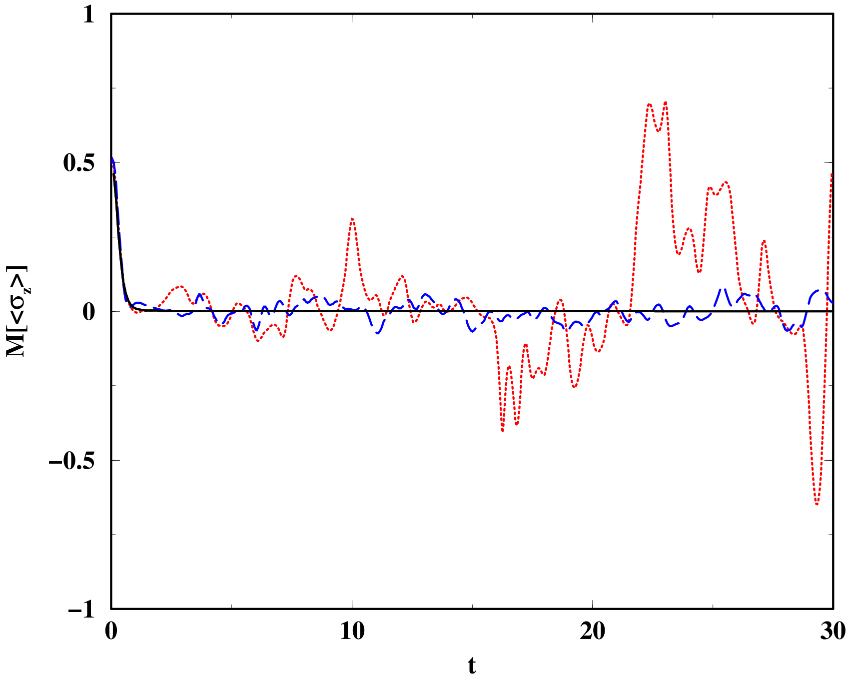

Fig. 5.4 Solutions of the *linear equation* (5.13) (dashed line) and the *shifted equation* (5.50) (long dashed line) for $\beta = 0.01$ (high temperatures), using an ensemble of $\kappa = 100$ trajectories. Results are compared to the master equation (thick black line)

A further question shall be addressed next: Does a normalization of the wave function during the evolution still improve the statistics? To answer we compare in Fig. 5.6 the results of the *shifted equation* (5.50) and the *non-linear* (also shifted) equation (5.52), which evolves normalized states and has the following form for the present system,

$$\begin{aligned} \frac{\partial |\tilde{\psi}_1(z^*(t))\rangle}{dt} &= -iH_S |\tilde{\psi}_1(z^*(t))\rangle + \tilde{z}_t^* \left[|\tilde{\psi}_2(z^*(t))\rangle - \langle \sigma_x \rangle |\tilde{\psi}_1(z^*(t))\rangle \right] \\ &- \int_0^t d\tau \alpha(t-\tau) \left[e^{-i\Delta(\tau-t)} |\tilde{\psi}_1(z^*(t))\rangle + \langle \sigma_x \rangle e^{i\Delta(\tau-t)} |\tilde{\psi}_2(z^*(t))\rangle \right] \end{aligned}$$

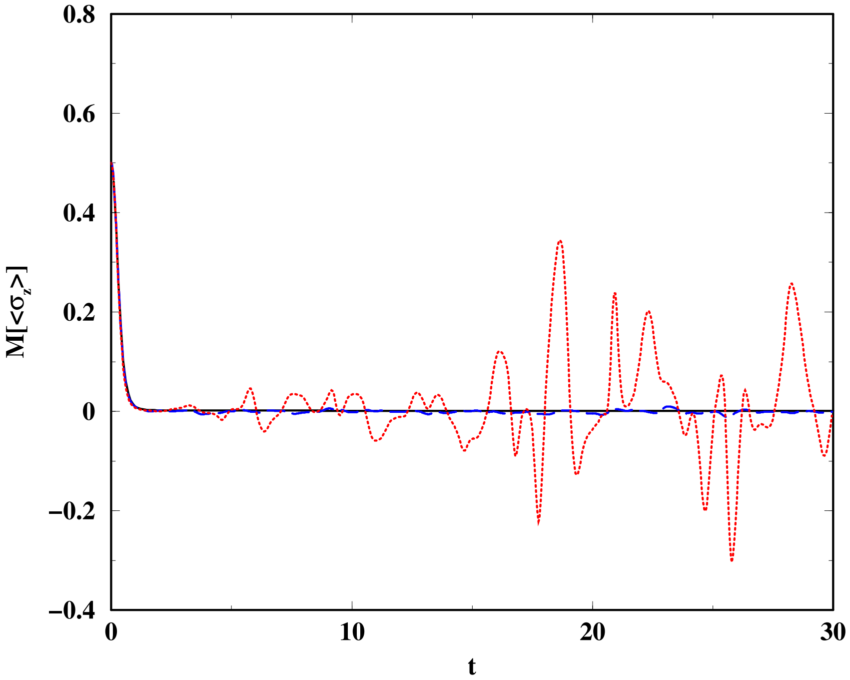

Fig. 5.5 Same as Fig. 5.4 but with $\kappa = 10000$ trajectories.

$$
\begin{aligned}
&+ \int_0^t d\tau\alpha(t-\tau)\Big[e^{-i\Delta(\tau-t)}\langle\tilde{\psi}_1(z^*(t))|\tilde{\psi}_1(z^*(t))\rangle \\
&+ e^{i\Delta(\tau-t)}\langle\tilde{\psi}_2(z^*(t))|\tilde{\psi}_2(z^*(t))\rangle\Big]|\tilde{\psi}_1(z^*(t))\rangle \\
&- \langle\sigma_x\rangle\int_0^t d\tau\alpha(t-\tau)\Big[e^{i\Delta(\tau-t)}\langle\tilde{\psi}_1(z^*(t))|\tilde{\psi}_2(z^*(t))\rangle \\
&+ e^{-i\Delta(\tau-t)}\langle\tilde{\psi}_2(z^*(t))|\tilde{\psi}_1(z^*(t))\rangle\Big]|\tilde{\psi}_1(z^*(t))\rangle
\end{aligned}
\tag{5.59}
$$

$$
\begin{aligned}
\frac{\partial|\tilde{\psi}_2(z^*(t))\rangle}{dt} &= iH_S|\tilde{\psi}_2(z^*(t))\rangle + \tilde{z}_t^*\left[|\tilde{\psi}_1(z^*(t))\rangle - \langle\sigma_x\rangle|\tilde{\psi}_2(z^*(t))\rangle\right] \\
&- \int_0^t d\tau\alpha(t-\tau)\Big[e^{i\Delta(\tau-t)}|\tilde{\psi}_2(z^*(t))\rangle + \langle\sigma_x\rangle e^{-i\Delta(\tau-t)}|\tilde{\psi}_1(z^*(t))\rangle\Big] \\
&+ \int_0^t d\tau\alpha(t-\tau)\Big[e^{-i\Delta(\tau-t)}\langle\tilde{\psi}_1(z^*(t))|\tilde{\psi}_2(z^*(t))\rangle \\
&+ e^{i\Delta(\tau-t)}\langle\tilde{\psi}_2(z^*(t))|\tilde{\psi}_2(z^*(t))\rangle\Big]|\tilde{\psi}_1(z^*(t))\rangle \\
&- \langle\sigma_x\rangle\int_0^t d\tau\alpha(t-\tau)\Big[e^{i\Delta(\tau-t)}\langle\tilde{\psi}_1(z^*(t))|\tilde{\psi}_2(z^*(t))\rangle \\
&+ e^{-i\Delta(\tau-t)}\langle\tilde{\psi}_2(z^*(t))|\tilde{\psi}_1(z^*(t))\rangle\Big]|\tilde{\psi}_2(z^*(t))\rangle,
\end{aligned}
\tag{5.60}
$$

where again $\tilde{z}_t^* = z_t^* + \int_0^t d\tau\alpha(t-\tau)\langle\sigma_x\rangle$, and $\langle\sigma_x\rangle = \langle\tilde{\psi}(z^*(t))|\sigma_z|\tilde{\psi}(z^*(t))\rangle$. Using an ensemble of $\kappa = 1000$ trajectories it appears that they both give the same degree of accuracy. To be more specific, for this number of trajectories it seems that the solutions of both equations still present some fluctuations around the result of the master equation, but these have the same amplitude in both cases. As a consequence, we can conclude that, at least for the spin-boson model, no further improvement of the statistics is achieved when averaging over the normalized solutions of equation (5.52). We conclude that in practice, it is irrelevant whether one normalizes after each time step. As long as one uses the shifted noise and keeps track of the norm in order to evaluate expectation values with the correct normalization factor, both the linear shifted equation (5.50) and the full nonlinear equation (5.52) give results of equal quality.

It is now important to study whether the *shifted equation* (5.50) still presents a better sampling than the *linear equation* (5.24) for low temperatures ($\beta = 10$). As shown by Gaspard and Nagaoka [35], the linear equation already gives averages that are in good agreement with the master equation. Figures 5.7 and 5.8 show that indeed, there is no appreciable improvement of the shifted equation with respect to the linear one in any of the two statistical ensembles of trajectories used (10000 and 150000 trajectories respectively). These results, added to the fact that the shifted equation is numerically slower, make the linear equation a more sensible choice in the low temperature regime.

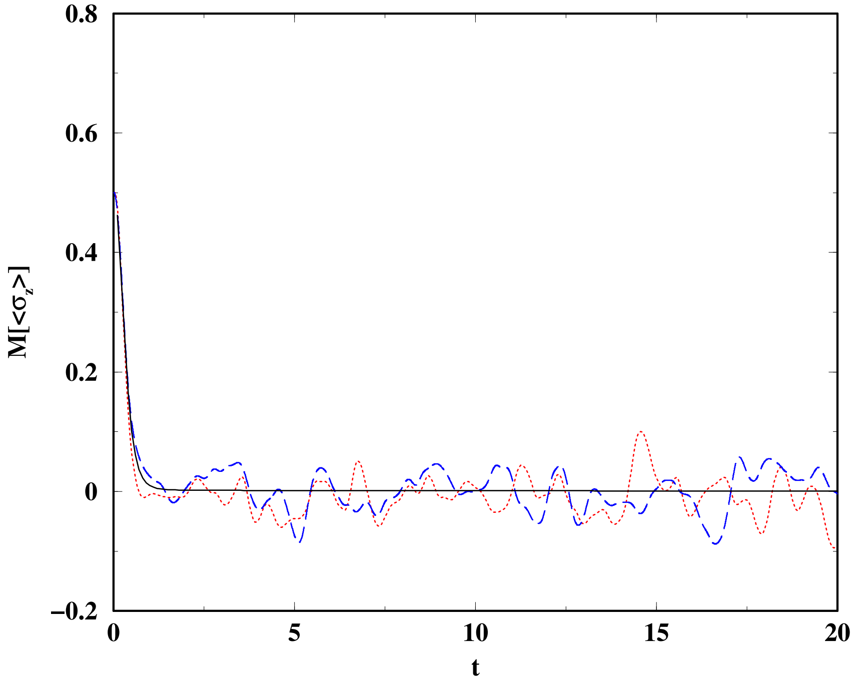

Fig. 5.6 Solutions of the *shifted equation* (5.50) and the *non-linear equation* (5.52) (long dashed and dotted line respectively) for $\beta = 0.01$ (high temperatures), with an average of $\kappa = 1000$ trajectories. The result of the master equation is displayed with a solid line.

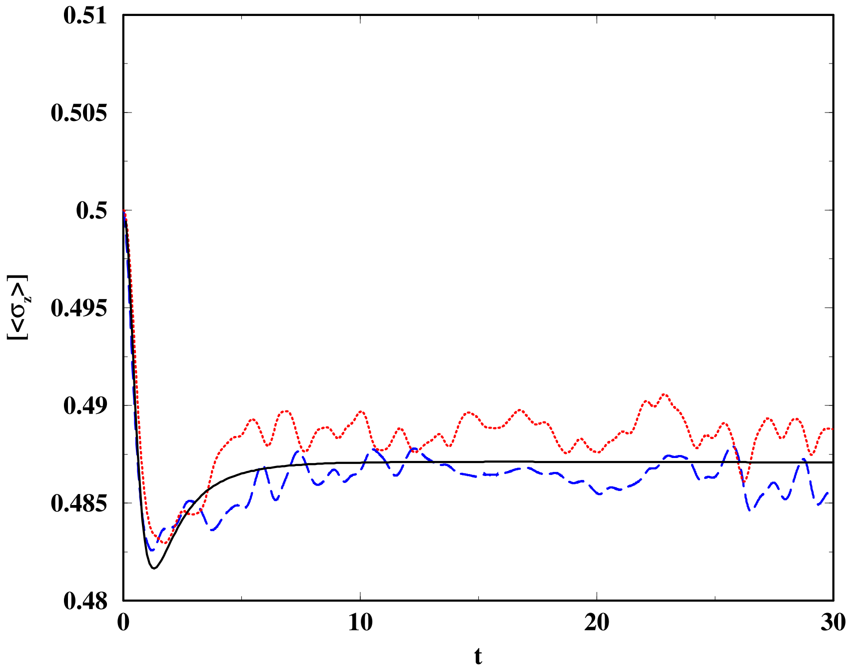

Fig. 5.7 Solutions of the *linear equation* (long dashed line) and the *shifted equation* (dotted line) for $\beta = 10$, averaged for 10000 trajectories. The results are compared to the one obtained from the master equation (thick black line).

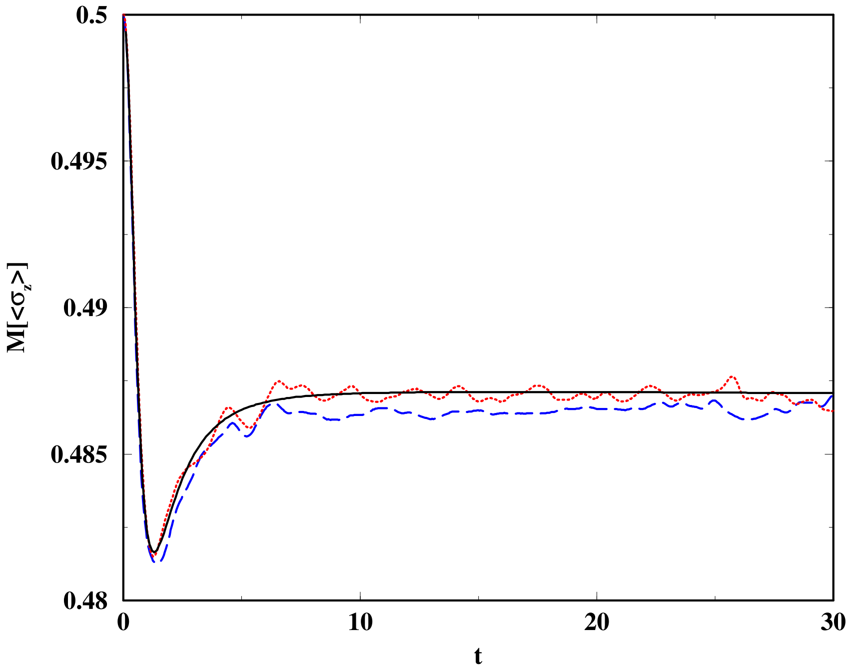

Fig. 5.8 Same as Fig. 5.7 but now with 150000 trajectories.

5.1.3.4 A study of the noise and the shifted noise When comparing the shift term in equation (5.49), $g\int_0^t d\tau\alpha(t-\tau)^*\langle{\sigma_x}^\dagger\rangle_\tau$, and the original noise z_t that appears in expression (5.49) for both temperature regimes, we find the reason for the previous observations. We present in Fig. 5.9 the time evolution of the real and imaginary parts of both quantities. For low temperatures $\beta = 10$, the shift remains close to zero during the whole evolution, and therefore its significance relative to the noise z_t is small. However, the situation changes for high temperatures, ($\beta = 0.01$), in which the real part of the shift reaches an amplitude of fluctuations equal to that of the noise, producing a shifted noise very distant from the non-shifted one.

These results can be seen more clearly in Figs. 5.10 and 5.11, which show the real and imaginary parts of the shift term and the noise for low and high temperatures, respectively. We observe that at low temperatures the region in which the shift is distributed (a black point located around the center of the coordinate system in Fig. 5.10) is small in comparison with the region of values of z_t. The situation at high temperatures is different, as we can see in Fig. 5.11. Here, the values of the shift term spreads horizontally across the real axis with magnitudes equal to those of the noise.

The latter results explain why at high temperatures it is essential to use the shifted noise equation (5.50), taking into account dynamically the dynamics of the probability distribution. For lower temperatures this shift is much less important, and the original *linear equation* can still be used satisfactorily.

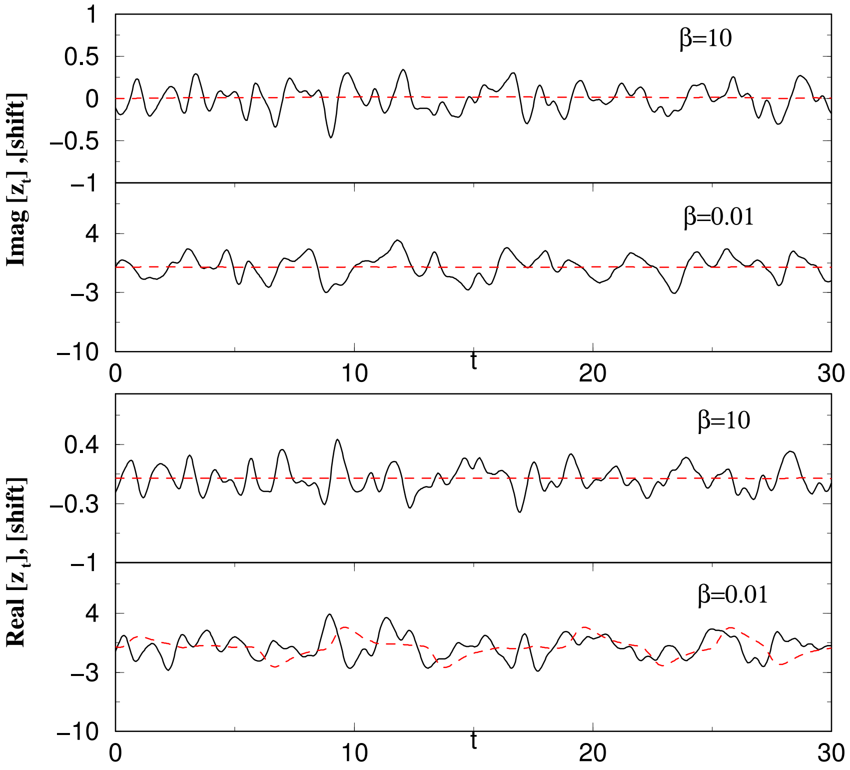

Fig. 5.9 Real and imaginary part of the noise (solid lines) and the shift term (dashed lines) as a function of time for both temperature regimes.

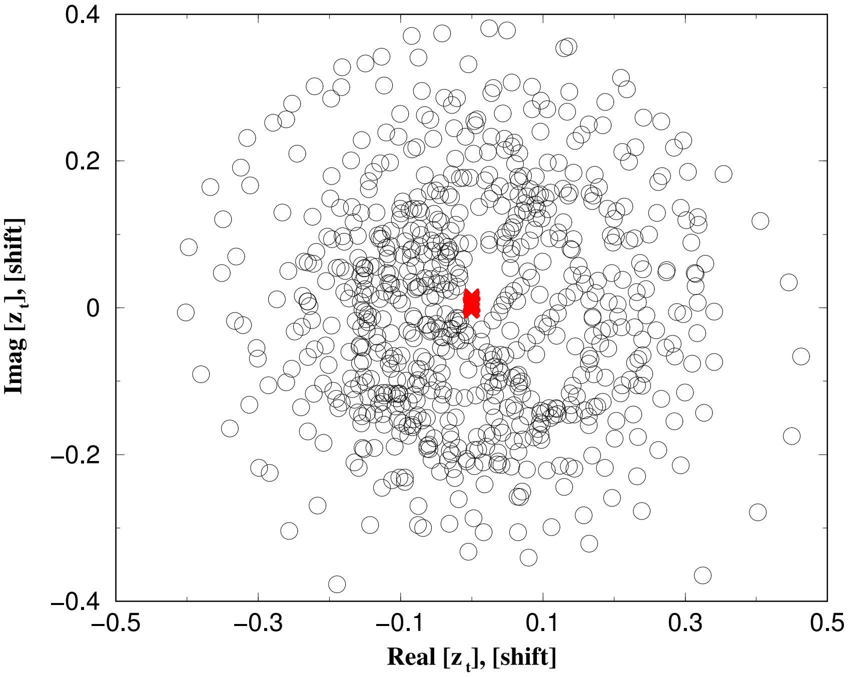

Fig. 5.10 Real and imaginary part of the noise (circles) and shift term (crosses) for low temperature, $\beta = 10$.

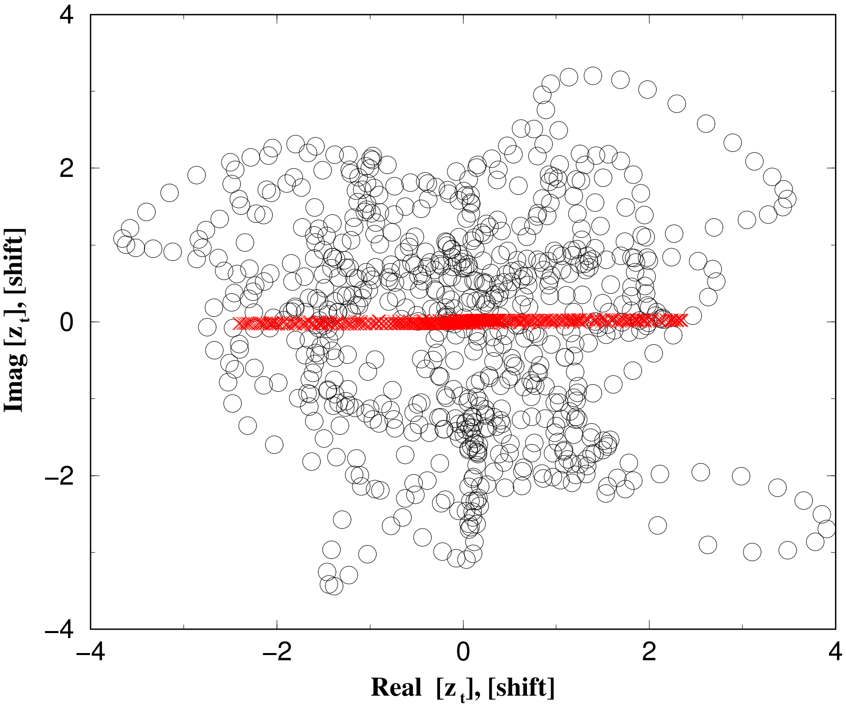

Fig. 5.11 Same as Fig. 5.10 but now for high temperature $\beta = 0.01$.

5.1.3.5 Noise and shift for other temperatures. Let us study the time averaged magnitude of the shift term in comparison to that of the noise for other temperature values. Here we define the time averaged magnitude of a stochastic quantity $f(t)$ simply as $T[f] = \frac{1}{T}\int_0^T d\tau |f(\tau)|$. The relation between these values will again give us an idea of the necessity of using a non-linear equation instead of the linear one. For intermediate temperatures (for values of β between 0.01 and 10) we see in Fig. 5.12 that only for very high temperatures (values of β close to zero), the magnitude of the real part of the shift is comparable to that of the noise, and therefore a non-linear equation is needed. However, for β greater than 0.1, even the real part of the shift term saturates to magnitudes very close to zero in comparison to the magnitude of the noise, which saturates to values of approximately 100 (in inverse time units).

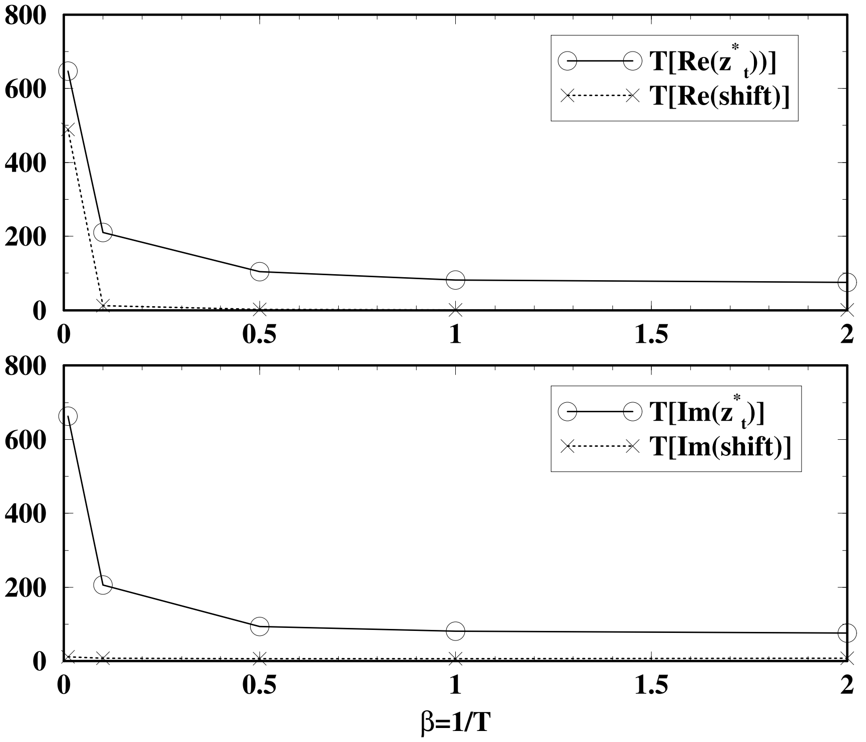

Fig. 5.12 Real and imaginary part of the time average (denoted as $T[*]$) of the absolute value of the noise (solid line with circles) and shift term (dotted line with crosses) for different inverse temperatures β. Only for very high temperatures the time average of the shift is relevant in comparison to the non-shifted noise.

5.2 REDUCED PROPAGATOR AS A TOOL TO DERIVE MASTER EQUATIONS

We show in this part different derivations of the master equation, according to different possible initial conditions for $\rho_{tot}(t)$. In order to obtain closed equations, we use the evolution equation of the reduced propagator up to second order in the perturbative parameter,

$$\begin{aligned}\frac{dG(z_i^* z_{i+1}|t0)}{dt} &= -iH_S G(z_i^* z_{i+1}|t0) + Lz_t^* G(z_i^* z_{i+1}|t0) - L^\dagger z_{i+1,t} G(z_i^* z_{i+1}|t0) \\ &- L^\dagger \int_0^t d\tau \alpha(t-\tau) V_{\tau-t} L G(z_i^* z_{i+1}|t0) + \mathcal{O}(g^3). \end{aligned} \quad (5.61)$$

with $z_{i+1} = z_0$ and $z_i = z$.

5.2.1 Dissipative master equation with decorrelated initial condition

Let us start by deriving the master equation of an initially decorrelated state $\rho_{tot}(0) = \rho_s(0) \otimes \rho_B$ for two cases: $\rho_B = |0\rangle\langle 0|$, and $\rho_B = \int d\mu(z_0) P(z_0^*, z_0)|z_0\rangle\langle z_0|$.

5.2.1.1 Zero temperature Let us here derive a master equation up to order g^2 in coupling constant for $\rho_B = |0\rangle\langle 0|$. We define the projector $\mathcal{P}_t(z_t^* z_t) \equiv \mathcal{P}_t = |\psi_t(z^*)\rangle\langle\psi_t(z)| = G(z^*0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(0z|0t)$, so that $\dot{\rho}_t = \mathcal{M}[\dot{\mathcal{P}}_t]$, and

$$\frac{d\mathcal{P}_t}{dt} = \frac{d|\psi_t(z^*)\rangle}{dt}\langle\psi_t(z)| + |\psi_t(z^*)\rangle\frac{d\langle\psi_t(z)|}{dt}. \tag{5.62}$$

In order to perform the average, it will be necessary to use the following properties,

$$\begin{aligned}\mathcal{M}[\mathcal{P}_t z_t] &= \int_0^t d\tau \mathcal{M}[z_t z_\tau^*] M\left[\frac{\delta \mathcal{P}_t}{\delta z_\tau^*}\right] \\ \mathcal{M}[\mathcal{P}_t z_t^*] &= \int_0^t d\tau \mathcal{M}[z_t^* z_\tau] M\left[\frac{\delta \mathcal{P}_t}{\delta z_\tau}\right],\end{aligned} \tag{5.63}$$

which hold for any complex Gaussian noise [54]. From the non-convoluted equation (5.61), with $z_0 = 0$, the time evolution (5.62) is

$$\begin{aligned}\frac{d\mathcal{P}_t}{dt} &= g z_t^* V_t L \mathcal{P}_t - g^2 V_t L^\dagger \int_0^t d\tau \alpha(t-\tau) V_\tau L \mathcal{P}_t + g z_t \mathcal{P}_t V_t L^\dagger \\ &- g^2 \mathcal{P}_t \int_0^t d\tau \alpha^*(t-\tau) V_\tau L^\dagger V_t L.\end{aligned} \tag{5.64}$$

Using equations (5.15) and (5.63), together with the fact that the wave function $|\psi_t(z^*)\rangle$ depends only on z^*, the ensemble average of the terms z_t in $\dot{\mathcal{P}}_t$ has been shown to be [54]:

$$\begin{aligned}\mathcal{M}[\mathcal{P}_t z_t^*] &= \int_0^t d\tau \mathcal{M}[z_t^* z_\tau] M\left[|\psi_t(z^*)\rangle \frac{\delta\langle\psi_t(z)|}{\delta z_\tau}\right] \\ &= \int_0^t d\tau \mathcal{M}[z_t^* z_\tau] \rho_t O^\dagger(t,\tau,z), \\ \mathcal{M}[\mathcal{P}_t z_t] &= \int_0^t d\tau \mathcal{M}[z_t z_\tau^*] M\left[\frac{\delta|\psi_t(z^*)\rangle}{\delta z_\tau^*}\langle\psi_t(z)|\right] \\ &= \int_0^t d\tau \mathcal{M}[z_t z_\tau^*] O(t,\tau,z)\rho_t.\end{aligned} \tag{5.65}$$

Performing the average of (5.64) with the use of the former properties, a (non-convoluted) second order master equation is obtained

$$\begin{aligned}\frac{d\rho_t}{dt} &= g^2 V_t L \rho_t \int_0^t d\tau \alpha^*(t-\tau) V_\tau L^\dagger + g^2 \int_0^t d\tau \alpha(t-\tau) V_\tau L \rho_t V_t L^\dagger \\ &- g^2 V_t L^\dagger \int_0^t d\tau \alpha(t-\tau) V_\tau L \rho_t - g^2 \rho_t \int_0^t d\tau \alpha^*(t-\tau) V_\tau L^\dagger V_t L.\end{aligned} \tag{5.66}$$

There is a convoluted version of (5.61) that is equivalent up to the same order

$$\begin{aligned}\frac{dG(z^*z_0|t0)}{dt} &= -iH_SG(z^*z_0|t0)+Lz_t^*G(z^*z_0|t0)-L^\dagger z_{0,t}G(z^*z_0|t0)\\ &- L^\dagger\int_0^t d\tau\alpha(t-\tau)V_{\tau-t}LG(z^*z_0|\tau 0)+\mathcal{O}(g^3),\end{aligned} \tag{5.67}$$

and it corresponds to the stochastic equation (5.20) when $z_0=0$ and z_t is interpreted as a noise. Inserting this equation into (5.62),

$$\begin{aligned}\frac{d\mathcal{P}_t}{dt} &= gz_t^*V_tL\mathcal{P}_t-g^2V_tL^\dagger\int_0^t d\tau\alpha(t-\tau)V_\tau L|\psi_\tau(z^*)\rangle\langle\psi_t(z)|\\ &+ gz_t\mathcal{P}_tV_tL^\dagger-g^2\int_0^t d\tau\alpha^*(t-\tau)|\psi_t(z^*)\rangle\langle\psi_\tau(z)|V_\tau L^\dagger V_tL,\end{aligned} \tag{5.68}$$

and then performing again an average over the variable z, a second order convoluted master equation can be obtained. Since the dissipative terms are already of second order, we can follow the same argument as in the previous section and consider the perturbative integration of the wave function, (this time from τ to t), only up to order zero. Under this assumption, $|\psi_t\rangle=|\psi_\tau\rangle+\mathcal{O}(g)$ and $\langle\psi_t|=\langle\psi_\tau|+\mathcal{O}(g)$. We can therefore consider, $|\psi_\tau\rangle\langle\psi_t|=|\psi_t\rangle\langle\psi_\tau|=\mathcal{P}_\tau+\mathcal{O}(g)$. The functional derivative in (5.63) is now directly performed in the analytic form of the projector $\mathcal{P}_t$ obtained from the perturbative integration of the last equation,

$$\begin{aligned}\mathcal{P}_t-\mathcal{P}_0 &= g\int_0^t d\tau V_\tau Lz_\tau^*\mathcal{P}_0+g\int_0^t\mathcal{P}_0V_\tau L^\dagger z_\tau d\tau\\ &+ g^2\int_0^t d\tau V_\tau Lz_\tau^*\int_0^\tau d\tau' V_{\tau'}Lz_{\tau'}^*\mathcal{P}_0\\ &+ g^2\int_0^t d\tau\left[\int_0^\tau d\tau' V_{\tau'}Lz_{\tau'}^*\mathcal{P}_0\right]V_\tau L^\dagger z_\tau\\ &- g^2\int_0^t d\tau V_\tau L^\dagger\int_0^\tau d\tau'\alpha(\tau-\tau')V_{\tau'}L\mathcal{P}_0\\ &- g^2\int_0^t d\tau\left[\int_0^\tau d\tau'\alpha^*(\tau-\tau')\mathcal{P}_0V_{\tau'}L^\dagger\right]V_\tau L+\mathcal{O}(g^3).\end{aligned} \tag{5.69}$$

Keeping terms only up to g^0, we find

$$\begin{aligned}\frac{\delta\mathcal{P}_t}{\delta z_\tau^*} &= V_\tau L\mathcal{P}_0+\mathcal{O}(g),\\ \frac{\delta\mathcal{P}_t}{\delta z_\tau} &= \mathcal{P}_0V_\tau L^\dagger+\mathcal{O}(g).\end{aligned} \tag{5.70}$$

As before, we can consider the zero order term of an expansion of the type (5.69), so that $\mathcal{P}_0=\mathcal{P}_t+\mathcal{O}(g)$ or $\mathcal{P}_0=\mathcal{P}_\tau+\mathcal{O}(g)$. Choosing the second possibility, and after the average, we find the following convoluted master equation:

$$\begin{aligned}\frac{d\rho_t}{dt} &= g^2V_tL\int_0^t d\tau\alpha^*(t-\tau)\rho_\tau V_\tau L^\dagger+g^2\int_0^t d\tau\alpha(t-\tau)V_\tau L\rho_\tau V_tL^\dagger\\ &- g^2V_tL^\dagger\int_0^t d\tau\alpha(t-\tau)V_\tau L\rho_\tau-g^2\int_0^t d\tau\rho_\tau\alpha^*(t-\tau)V_\tau L^\dagger V_tL.\end{aligned} \tag{5.71}$$

To summarize, the second order equations (5.61) and (5.67) (which correspond respectively to (5.13) and (5.20)) have been used to obtain a convoluted and a non-convoluted master equation respectively. The method is based on solving perturbatively the dynamical equations of $|\psi_t\rangle$ and $\mathcal{P}_t$. The fact that all the integral terms appearing in the equations are already of second order (so that it is equivalent to consider in them $|\psi_0\rangle = |\psi_t\rangle + \mathcal{O}(g)$ or $|\psi_0\rangle = |\psi_\tau\rangle + \mathcal{O}(g)$, and analogously with $\mathcal{P}_0$), emphasizes that, up to this order, a convoluted equation is equivalent to a non-convoluted one. For that reason, a remarkable difference in the result derived from a convoluted and a non-convoluted equation will therefore indicate a failure in the second order perturbative approximation. This issue is discussed with further detail in Chapter (IV) for a two level atom in a PBG material.

5.2.1.2 Non-zero temperature As mentioned Section (2.2), the propagator with evolution given by (5.61) permits us to calculate the master equation for a system with $\rho_s(0) = |\psi_0\rangle\langle\psi_0|$ coupled to an environment represented by a general P coherent distribution, in such a way that $\rho_{tot}(0) = \int d\mu(z_0)P(z_0, z_0^*)|\psi_0\rangle|z_0\rangle\langle z_0|\langle\psi_0|$. This density matrix evolves in time as follows,

$$\rho_{tot}(t) = \int d\mu(z_0)P(z_0, z_0^*)\mathcal{U}_I(t,0)|z_0\rangle|\psi_0\rangle\langle\psi_0|\langle z_0|\mathcal{U}_I^{-1}(t,0). \tag{5.72}$$

Inserting twice the identity of the Bargmann representation, the former expression can be written as

$$\begin{aligned}\rho_{tot}(t) &= \int d\mu(z_2)\int d\mu(z_1)\int d\mu(z_0)P(z_0, z_0^*)\langle z_1|\mathcal{U}_I(t,0)|z_0\rangle|\psi_0\rangle \\ &\quad \langle\psi_0|\langle z_0|\mathcal{U}_I^{-1}(t,0)|z_2\rangle|z_1\rangle\langle z_2|,\end{aligned} \tag{5.73}$$

which shows that although system and environment might be initially decorrelated, they become correlated during the interaction. The reduced density matrix of the system, which is defined as $\rho_s = Tr_B\left(\rho_{tot}\right)$ is equal to,

$$\rho_s(t) = \int d\mu(z_0)P(z_0, z_0^*)\rho_s(z_0^*z_0|t), \tag{5.74}$$

where we have made the following definition,

$$\rho_s(z_0^*z_0|t) = \int d\mu(z_1)G(z_1^*z_0|t0)\rangle|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^*z_1|0t). \tag{5.75}$$

The evolution of $\rho_s(z_0^*z_0|t)$ is given by

$$\frac{d\rho_s(z_0^*z_0|t)}{dt} = \frac{d}{dt}\mathcal{M}_1\left[G(z_1^*z_0|t0)|\psi\rangle\langle\psi|G^\dagger(z_0^*z_1|0t)\right]. \tag{5.76}$$

If we insert in the former expression the second order perturbative evolution equation (5.61), as well as its complex conjugated version, it becomes

$$\begin{aligned}\frac{d\rho_s(z_0^*z_0|t)}{dt} &= -i[H_S, \rho_s(z_0^*z_0|t)] - z_{0,t}L^\dagger\rho_s(z_0^*z_0|t) - z_{0,t}'^*\rho_s(z_0^*z_0|t)L \\ + & \int_0^t d\tau\alpha(t-\tau)L^\dagger V_{\tau-t}L\rho_s(z_0^*z_0|t) - \int_0^t d\tau\alpha^*(t-\tau)\rho_s(z_0^*z_0|t)V_{t-\tau}L^\dagger L \\ + & \mathcal{M}_1\left[z_{1,t}G(z^*z_0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^*z_1|t0)L^\dagger\right] \\ + & \mathcal{M}_1\left[z_{1,t}^*LG(z_1^*z_0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^*z_1|t0)\right] + \mathcal{O}(g^3).\end{aligned} \tag{5.77}$$

In order to perform the average in z_1, it is necessary to take into account that the initial condition of the functional appearing inside the corresponding terms is

$$G(z_1^* z_0|00)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^* z_1|00) = e^{(z_1^* z_0)} e^{(z_0^* z_1)}|\psi_0\rangle\langle\psi_0|. \tag{5.78}$$

In that case, the average cannot be made using the property (5.65). Instead, we have to use the property

$$\begin{aligned} \mathcal{M}_i\left[z_{i,t_i}\mathcal{W}[t_i,t_{i+1}]\right] &= z_{i+1,t_i}\mathcal{M}_i\left[\mathcal{W}[t_i,t_{i+1}]\right] \\ + & \int_{t_{i+1}}^{t_i} d\tau \mathcal{M}_i\left[z_{i,t}z_{i,\tau}^*\right]\mathcal{M}_i\left[\left(\frac{\delta\mathcal{W}[t_i,t_{i+1}]}{\delta z_{i,\tau}^*}\right)\right], \end{aligned} \tag{5.79}$$

obtained in Appendix (I) for the average of z_{i,t_i} with general functionals $\mathcal{W}[t_i,t_{i+1}]$ with initial condition $\exp\left(z_i^* z_{i+1}\right)$. Then, the average of the noise term $z_{1,t}$ is the following [1]

$$\begin{aligned} \mathcal{M}\left[z_{1,t}G(z_1^* z_0|t0)|\psi_0(z_0)\rangle\langle\psi_0(z_0)|G^\dagger(z_0'^* z_1|0t)L^\dagger\right] &= z_{0t}\rho_s(z_0 z_0^*|t)L^\dagger \\ + & \int_0^t d\tau\alpha(t-\tau)V_{\tau-t}L\rho_s(z_0 z_0^*|t)L^\dagger + \mathcal{O}(g^3), \end{aligned} \tag{5.80}$$

where we have considered that $\frac{\delta G(z_1^* z_0|t0)}{\delta z_{1,\tau}^*} = V_{\tau-t}LG(z_1^* z_0|t0)$ In the same way we have,

$$\begin{aligned} \mathcal{M}\left[z_{1,t}^* LG(z_1^* z_0|t0)|\psi_0(z_0)\rangle\langle\psi_0(z_0)|G^\dagger(z_0^* z_1|0t)\right] &= z_{0t}^* L\rho_s(z_0^* z_0|t) \\ + & L\rho_s(z_0^* z_0|t)\int_0^t d\tau\alpha^*(t-\tau)V_{\tau-t}L^\dagger + \mathcal{O}(g^3). \end{aligned} \tag{5.81}$$

Inserting (5.80) and (5.81) in (5.73), we have the following second order master equation for $\rho_s(z_0^* z_0|t)$,

$$\begin{aligned} \frac{d\rho_s(z_0^* z_0|t)}{dt} &= -i[H_S,\rho_s(z_0^* z_0|t)] + z_{0,t}[\rho_s(z_0^* z_0|t),L^\dagger] \\ + & z_{0,t}^*[L,\rho_s(z_0^* z_0|t)] + \int_0^t d\tau\alpha(t-\tau)[V_{\tau-t}L\rho_s(z_0^* z_0|t),L^\dagger] \\ + & \int_0^t d\tau\alpha^*(t-\tau)[L,\rho_s(z_0^* z_0|t)V_{\tau-t}L^\dagger] + \mathcal{O}(g^3). \end{aligned} \tag{5.82}$$

Let us now perform the average of (5.82) with respect to z_0. The terms with $z_{0,t}$ and $z_{0,t}^*$ are of order g. For that reason, in order to obtain a second order perturbative master equation, it is necessary to compute their average by inserting first order perturbative expansion of $\rho(z_0^* z_0)$, which is given by (J.7) as,

$$\begin{aligned} \rho_s(z_0^* z_0|t) &= \int d\mu(z_1)G(z_1^* z_0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^* z_1) \\ &= e^{z_0^* z_0}\Big(\rho_s(z_0^* z_0|t) + \int_0^t d\tau z_{0,\tau}^*[V_{\tau-t}L,\rho_s(z_0^* z_0|t)] \\ &+ \int_0^t d\tau z_{0,\tau}[\rho_s(z_0^* z_0|t),V_{\tau-t}L^\dagger]\Big) + \mathcal{O}(g^2). \end{aligned} \tag{5.83}$$

---

[1] Such properties can be derived within a second order perturbative approximation, as shown in Appendix (J)

If we now chose the $P(z_0,z_0^*)$ as the P distribution of a thermal reservoir,

$$P(z_0,z_0^*)=\prod_\lambda \frac{1}{\pi N(\omega_\lambda)}e^{-|z_0|^2 N(\omega_\lambda)}, \tag{5.84}$$

it can be easily checked that

$$\begin{aligned}\mathcal{M}_0[z_{0t}\rho_s(z_0^*z_0|t)] &= -\int d\mu(z)\int d\mu(z_0)P(z_0,z_0^*)e^{z_0z^*+zz_0^*}\int_0^t d\tau z_{0t}z_{0\tau}^*[V_{\tau-t}L,|\psi_0\rangle\langle\psi_0|]\\ &= -\int_0^t d\tau\alpha^{+*}(\tau-t)[V_{\tau-t}L,\rho_s(t)]+\mathcal{O}(g^3).\end{aligned} \tag{5.85}$$

Then the average of the second term of (5.82) is

$$\mathcal{M}_0[z_{0t}\rho_s(z_0^*z_0|t)] = \int_0^t d\tau\alpha^{+*}(\tau-t)[\rho_s(t),V_{\tau-t}L^\dagger]. \tag{5.86}$$

We have here defined the funtion $\alpha^+(t-\tau)$ as in (4.21). Where, as before, $N(\omega_\lambda)$ is the average thermal number of quanta in the mode ω_λ, defined in terms of the temperature $\beta=1/\kappa_BT$ as $N(\omega)=[\exp(\omega\beta)-1]^{-1}$. After a replacement of (5.85) and (5.86), the average of (5.82) over z_0 is

$$\begin{aligned}\frac{d\rho_s(t)}{dt} &= -i[H_S,\rho_s(t)]+\int_0^t d\tau\alpha^{+*}(t-\tau)[[V_{\tau-t}L,\rho_s(t)],L^\dagger]\\ &+ \int_0^t d\tau\alpha^{+}(t-\tau)[L,[\rho_s(t),V_{\tau-t}L^\dagger]]\\ &+ \int_0^t d\tau\alpha(t-\tau)[V_{\tau-t}L\rho_s(t),L^\dagger]\\ &+ \int_0^t d\tau\alpha^{*}(t-\tau)[L,\rho_s(t)V_{\tau-t}L^\dagger]+\mathcal{O}(g^3).\end{aligned} \tag{5.87}$$

Let us now define the correlation function $\alpha^-(t-\tau)$ defined in (4.20). In terms of such correlation, the former equation becomes like (4.19),

$$\begin{aligned}\frac{d\rho_s(t)}{dt} &= -i[H_S,\rho_s(t)]+\int_0^t d\tau\alpha^{+*}(t-\tau)[L^\dagger,\rho_s(t)V_{\tau-t}L]\\ &+ \int_0^t d\tau\alpha^{+}(t-\tau)[V_{\tau-t}L^\dagger\rho_s(t),L]\\ &+ \int_0^t d\tau\alpha^{-}(t-\tau)[V_{\tau-t}L\rho_s(t),L^\dagger]\\ &+ \int_0^t d\tau\alpha^{-*}(t-\tau)[L,\rho_s(t)V_{\tau-t}L^\dagger]+\mathcal{O}(g^3).\end{aligned} \tag{5.88}$$

This equation is the same as the one obtained by Gaspard and Nagaoka in [35, 37] [2], and the one obtained by making an ensemble average of the equation (5.21) derived by Diósi, Gisin and Strunz in [40].

---

[2] Which is identical to equation (4.16), considering (5.29) and (5.28) as the environment and system operators, and identifying the correlation functions $\alpha^{(\pm)}=2\,(C_{11}\pm C_{21})$.

5.3 DISSIPATIVE MASTER EQUATION WITH CORRELATED INITIAL CONDITIONS

As mentioned in the introduction, the propagator with evolution given by (5.61) permits us to calculate master equations with general initial conditions. Suppose for instance that we have a *pure* initial state for the total density matrix,

$$\rho_{tot}(0) = |\Psi_0\rangle\langle\Psi_0| = \int d\mu(z_0) \int d\mu(z_0')|z_0\rangle|\psi_0(z_0^*)\rangle\langle\psi_0(z_0')|\langle z_0'|. \tag{5.89}$$

In order to obtain physical results, this state should be normalized as $\rho_{tot}(0) = |\Psi_0\rangle\langle\Psi_0|/\langle\Psi_0|\Psi_0\rangle$. For simplicity, we will omit in the calculus that follows the normalization factor, although it will be taken into account in the initial condition of the examples we show in the next sections. Then the total density matrix reads as follows,

$$\rho_{tot}(t) = \int d\mu(z_0) \int d\mu(z_0')\mathcal{U}_I(t,0)|z_0\rangle|\psi_0(z_0^*)\rangle\langle\psi_0(z_0')|\langle z_0'|\mathcal{U}_I^{-1}(t,0). \tag{5.90}$$

The reduced density matrix of the system, which is defined as $\rho_s = Tr_B\{\rho_{tot}\}$ is equal to,

$$\rho_s(t) = \int d\mu(z_0) \int d\mu(z_0')\rho_s(z_0'^* z_0' z_0^* z_0|t), \tag{5.91}$$

where we have made the following definition,

$$\rho_s(z_0'^* z_0' z_0^* z_0|t) = \int d\mu(z_1)G(t0|z_1^* z_0))|\psi_0(z_0^*)\rangle\langle\psi_0(z_0')|G^\dagger(t0|z_0'^* z_1). \tag{5.92}$$

Once $\rho_s(z_0'^* z_0' z_0^* z_0|t)$ is known, then the sum (5.91) can be performed in order to obtain the reduced density operator. This may be done for each particular initial condition, which is given by the set of values $|\psi_0(z_0^*)\rangle$ for each z_0. Hence, it is interesting to compute the evolution equation of $\rho_s(z_0'^* z_0' z_0^* z_0|t)$, since it represents the most general object needed to compute ρ_s. Such evolution,

$$\frac{d\rho_s(z_0'^* z_0' z_0^* z_0|t)}{dt} = \frac{d}{dt}M_1\left[G(z_1^* z_0|t0)|\psi(z_0)\rangle\langle\psi(z_0')|G^\dagger(z_0'^* z_1|t0)\right], \tag{5.93}$$

can obtained within the perturbative approximation by using equation (5.61) for the propagator. In that way equation (5.93) becomes

$$\begin{aligned}
\frac{d\rho_s(z_0'^* z_0' z_0^* z_0|t)}{dt} &= -i[H_S, \rho_s(z_0'^* z_0' z_0^* z_0|t)] - z_{0,t}L^\dagger\rho_s(z_0'^* z_0' z_0^* z_0|t) - z_{0,t}'^*\rho_s(z_0'^* z_0' z_0^* z_0|t)L \\
+ & \int_0^t d\tau\alpha(t-\tau)L^\dagger V_{\tau-t}L\rho_s(z_0'^* z_0' z_0^* z_0|t) - \int_0^t d\tau\alpha^*(t-\tau)\rho_s(z_0'^* z_0' z_0^* z_0|t)V_{t-\tau}L^\dagger L \\
+ & \mathcal{M}_1\left[z_{1,t}^* LG(z_1^* z_0|t0)|\psi_0(z_0^*)\rangle\langle\psi_0(z_0')|G^\dagger(z_0'^* z_1|t0)\right] \\
+ & \mathcal{M}_1\left[z_{1,t}G(z_1^* z_0|t0)|\psi_0(z_0^*)\rangle\langle\psi_0(z_0')|G^\dagger(z_0'^* z_1|t0)L^\dagger\right] + \mathcal{O}(g^3),
\end{aligned} \tag{5.94}$$

where we stress again that the initial condition should be normalized

$$\rho_s(z_0'^* z_0' z_0^* z_0|0) = |\psi_0(z_0^*)\rangle\langle\psi_0(z_0')|/(\exp(z_0'^* z_0)\langle\psi_0(z_0')||\psi_0(z_0^*)\rangle. \tag{5.95}$$

In order to obtain the master equation up to second order in the perturbative parameter, we can use the perturbative expansion

$$\begin{aligned} G(z_1^*, z_0|t_1 0) = & \left\{ 1 + \int_0^{t_1} d\tau z_{1,\tau}^* V_{\tau - t_1} L - \int_0^{t_1} d\tau z_{0,\tau} V_{\tau - t_1} L^\dagger \right. \\ - & \int_0^{t_1} d\tau \int_t^\tau d\tau' \alpha(\tau - \tau') V_{\tau - t_1} L^\dagger V_{\tau' - t_1} L + \int_t^{t_1} d\tau \int_t^\tau d\tau' z_{1,\tau}^* z_{1,\tau'}^* V_{\tau - t_1} L V_{\tau' - t_1} L \\ - & \int_t^{t_1} d\tau \int_0^\tau d\tau' z_{1,\tau}^* z_{0,\tau'} V_{\tau - t_1} L V_{\tau' - t_1} L^\dagger - \int_0^{t_1} d\tau \int_0^\tau d\tau' z_{0,\tau} z_{1,\tau'}^* V_{\tau - t_1} L^\dagger V_{\tau' - t_1} L \\ - & \left. \int_0^{t_1} d\tau \int_0^\tau d\tau' z_{0,\tau} z_{0,\tau'} V_{\tau - t_1} L^\dagger V_{\tau' - t_1} L^\dagger \right\} G^{(}0)(z_1^* z_0|t_1 0) + \mathcal{O}(g^3), \end{aligned} \tag{5.96}$$

considering now $t = 0$ and the proper labels for the noises. Such expansion can be inserted in the average of the noise term z_t,

$$\mathcal{M}_1 \left[z_{1,t} G(z_1^* z_0|t0) |\psi_0(z_0^*)\rangle \langle \psi_0(z_0')| G^\dagger(z_0'^* z_1|t0) L^\dagger \right], \tag{5.97}$$

to find that, up to second order (see Appendix (J) for details),

$$\begin{aligned} \mathcal{M}_1 \left[z_{1,t} G(z_1^* z_0|t0) |\psi_0(z_0^*)\rangle \langle \psi_0(z_0')| G^\dagger(z_0'^* z_1|t0) L^\dagger \right] &= z_{0,t} \rho_s(z_0'^* z_0' z_0^* z_0|t) L^\dagger \\ + \int_0^t d\tau \alpha(t - \tau) V_{\tau - t} L \rho_s(z_0'^* z_0' z_0^* z_0|t) L^\dagger + \mathcal{O}(g^3). & \end{aligned} \tag{5.98}$$

In the last expression, we have replaced the first order density operator in perturbation parameter

$$\begin{aligned} \rho_s^{(1)}(z_0'^* z_0' z_0^* z_0|t) &= \rho_s^{(0)}(z_0'^* z_0' z_0^* z_0|t) + \int_0^t d\tau z_{0,\tau}'^* [V_{\tau - t} L, \rho_s^{(0)}(z_0'^* z_0' z_0^* z_0|t)] \\ &+ \int_0^t d\tau z_{0,\tau} [\rho_s^{(0)}(z_0'^* z_0' z_0^* z_0|t), V_{\tau - t} L^\dagger], \end{aligned} \tag{5.99}$$

by $\rho_s(z_0'^* z_0' z_0^* z_0|t)$, since it appears in terms which are at least of first order in g. Note that the last expression is in terms of the zero order density operator

$$\rho_s^{(0)}(z_0'^* z_0' z_0^* z_0|t) = e^{-iH_S t} |\psi_0(z_0)\rangle \langle \psi_0(z_0')| e^{iH_S t} e^{z_0'^* z_0}. \tag{5.100}$$

In the same way we have,

$$\begin{aligned} \mathcal{M}_1 \left[z_{1,t}^* L G(z^* z_0|t0) |\psi_0(z_0^*)\rangle \langle \psi_0(z_0')| G^\dagger(z_0'^* z_1|t0) \right] &= z_{0,t}'^* L \rho_s(z_0 z_0'^*|t0) \\ + L \rho_s(z_0'^* z_0' z_0^* z_0|t) \int_0^t d\tau \alpha^*(t - \tau) V_{\tau - t} L^\dagger + \mathcal{O}(g^3). & \end{aligned} \tag{5.101}$$

Inserting (5.98) and (5.101) in (5.94), we have the following second order master equation for $\rho_s(z_0 z_0'^*)$,

$$\begin{aligned} \frac{d\rho_s(z_0'^* z_0' z_0^* z_0|t)}{dt} &= -i[H_S, \rho_s(z_0'^* z_0' z_0^* z_0|t)] + z_{0,t}[\rho_s(z_0 z_0'^*), L^\dagger] + z_{0,t}'^*[L, \rho_s(z_0'^* z_0' z_0^* z_0|t)] \\ &+ \int_0^t d\tau \alpha(t - \tau)[V_{\tau - t} L \rho_s(z_0'^* z_0' z_0^* z_0|t), L^\dagger] \\ &+ \int_0^t d\tau \alpha^*(t - \tau)[L, \rho_s(z_0'^* z_0' z_0^* z_0|t) V_{\tau - t} L^\dagger] + \mathcal{O}(g^3). \end{aligned} \tag{5.102}$$

Suppose now that we have an initial *mixed state* for the total system, as defined in Section (2.2.2.2),

$$\rho_{tot}(0) = \int d\mu(z_0)\mathcal{J}(z_0, z_0^*)|\Psi_0(z_0^*)\rangle\langle\Psi_0(z_0)|, \tag{5.103}$$

where $\mathcal{J}(z_0, z_0^*)$ is the statistical probability for the member $|\Psi_0(z_0^*)\rangle$ of the statistical ensemble. Then, the reduced density matrix of the system, $\rho_s = Tr_B\{\rho_{tot}\}$ is equal to,

$$\rho_s(t) = \int d\mu(z_0)\mathcal{J}(z_0 z_0^*)\rho_s(z_0^* z_0|t), \tag{5.104}$$

which is equal to (5.91), but now with the following definition,

$$\rho_s(z_0^* z_0|t) = \int d\mu(z_1)G(t0|z_1^* z_0)\rangle|\psi_0(z_0^*)\rangle\langle\psi_0(z_0)|G^\dagger(t0|z_0^* z_1), \tag{5.105}$$

which is equal to (5.92), but with $z_0' = z_0$. Once such replacement is made, equation (5.102) represents the evolution of $\rho_s(z_0^* z_0|t)$. As in the pure case, provided that the whole set of initial conditions $|\psi_0(z_0^*)\rangle$ is known for the problem, as well as the probability distribution $\mathcal{J}(z_0, z_0^*)$ which describes its frequency in the mixture, then the sum (5.104) can be performed with the solutions $\rho_s(z_0^* z_0|t)$.

In the next sections, we are going to compute the evolution of $\rho_s(z_0'^* z_0' z_0^* z_0|t)$ with two examples, the solvable model with $L \propto H_S$, and the spin boson model. The evolution of $\rho_s(z_0^* z_0|t)$ is just a particular case of the former one. To this end, we will verify the equation (5.102) by comparing its results with those obtained by performing a numerical sampling over stochastic trajectories of the reduced propagator, following the relation (5.93).

It is clear that equation (5.102) is the essential piece for calculating the evolution equation of single mean values for general initial conditions. The next sections are devoted to prove such an equation by applying it to a model with $L = \sigma_z$ and $H_S = \omega_s\sigma_z/2$, which is analytically solvable, and to a spin-boson model.

5.3.1 A solvable model

We illustrate the equation (5.102) by applying it to a solvable model, where $L = \sigma_z$ and $H_S = \omega\sigma_z/2$. First of all, we calculate the mean value of an observable A that has, in the basis of eigenvectors of σ_z, the matrix representation $A = \begin{pmatrix} 0 & \alpha \\ \beta & 0 \end{pmatrix}$. Taking as the initial values for the states of the total system $|\Psi_0(z_0^*)\rangle = |\psi_0(z_0^*)\rangle|z_0\rangle$ and $|\Psi_0(z_0')\rangle = |\psi_0(z_0'^*)\rangle|z_0'?\rangle$, the average of A over these two vectors is given by

$$\langle\Psi_0(z_0')|A|\Psi_0(z_0^*)\rangle = \mathcal{M}_1\left[\langle\psi_0(z_0')|G^\dagger(z_0'^* z_1|0t)AG(z_1^* z_0|t0)|\psi_0(z_0^*)\rangle\right]. \tag{5.106}$$

In the present case, the solution of the equation (5.61) can simply be written as

$$\begin{aligned} G(z_1^* z_0|t_1 0) = \exp\Bigg\{ & -i\frac{\omega_S}{2}(t_1 - 0)\sigma_z + L\int_0^{t_1} d\tau z_{1,\tau}^* - L^\dagger \int_0^{t_1} d\tau z_{0,\tau}^* \\ - \quad & LL^\dagger \int_0^{t_1} d\tau \int_0^{\tau} ds\alpha(\tau - s) + z_1^* z_0 \Bigg\}. \end{aligned} \tag{5.107}$$

From the equation (5.107), performing the average over the environment degrees of freedom z_1 we obtain,

$$\langle A\rangle \quad = \quad e^{-2\int_0^t d\tau \int_0^\tau ds(\alpha(\tau-s)+\alpha^*(\tau-s))}\{\alpha\langle\psi_{0,1}|\psi_{0,2}\rangle e^{i\omega t+2\int_0^t d\tau(z_{0,\tau}-z_{0,\tau}'^*)}$$

$$+ \quad \beta\langle\psi_{02}|\psi_{01}\rangle e^{-i\omega t-2\int_0^t d\tau(z_{0,\tau}-z'^*_{0,\tau})}\}, \tag{5.108}$$

where we have taken a normalized initial system state $|\psi_0(z'^*_0)\rangle = |\psi_0\rangle = |\psi_{01}\rangle + |\psi_{02}\rangle$. In the same manner it follows for $\langle\sigma_z\rangle$

$$\langle\sigma_z\rangle = \langle\psi_{01}|\psi_{01}\rangle - \langle\psi_{02}|\psi_{02}\rangle. \tag{5.109}$$

Figure 5.13 represents (5.108) for $A = \sigma_i, i = x, y$, and (5.109) compared to the result obtained using the propagator (5.61). When the number of stochastic trajectories included in the ensemble mean (5.93) is large enough, both results coincide. The correlation function is obtained for 2 oscillators with coupling parameters $g_1 = g_2 = g = 0.1$, frequencies $\omega_1 = 6$ and $\omega_2 = 2$, and for an atom with rotating frequency $\omega_S = 4$.

5.3.2 A dissipative example: the spin-boson model

Let us now calculate the expectation value $\langle\Psi_0|A|\Psi_0\rangle$, where A is an operator belonging to the Hilbert space of a spin which is coupled to a thermal bath of harmonic oscillators, as described by the spin-boson model [35]. We consider the interaction Hamiltonian of (5.8) with a coupling operator $L = \sigma_x$, and a magnitude small enough to be considered perturbative. Within this model, the bath can be characterized by the spectral strength

$$J(\omega) = \frac{\omega^3}{\omega_c^2} e^{-\omega/\omega_c}, \tag{5.110}$$

where ω_c is a cutoff frequency [22, 34, 35, 37], here chosen as $\omega_c = 1$. The correlation function of the noise generated by a termal bath is given in terms of $J(\omega)$ as

$$\alpha(t) = \int_0^\infty d\omega J(\omega) \left[\coth\left(\frac{\omega\beta}{2}\right)\cos(\omega t) - i\sin(\omega t)\right]. \tag{5.111}$$

The inverse temperature $\beta = (\kappa_B T)^{-1}$ is chosen according to the energy of the bath, and considering that the energy of the subsystem is very small compared to it [35]. As noted when introducing the reduced propagator, when the environment is at high temperatures the noise statistics evolve quite significantly in time, so that a non-linear equation (see appendix (H)) needs to be considered in order to take this into account. On the contrary, for low temperatures the state distribution of the bath (i.e. the noise distribution), remains quite close to a Gaussian during the interaction, and linear equations are a good enough description of the problem. Since in our present case we consider low temperatures, $\beta = 10$, the linear stochastic equations for the propagators presented in this paper are suitable. In order to reduce the computational effort, we propose a Fourier expansion of (5.111) of the form

$$\alpha^{apprx}(t-\tau) = \sum_{m=-\nu/2}^{\nu/2} C(m) e^{-i\pi m(t-\tau)/T_{max}}, \tag{5.112}$$

with the coefficients

$$C(m) = \frac{1}{2T_{max}} \int_{-T_{max}}^{T_{max}} dt\alpha(t) e^{i\pi mt/T_{max}}. \tag{5.113}$$

where, T_{max} is the time window in which the correlation function is expanded in the series. With only $m = 6$ oscillators, the obtained correlation function is a good approximation of (5.111) up to $T = 5$. The

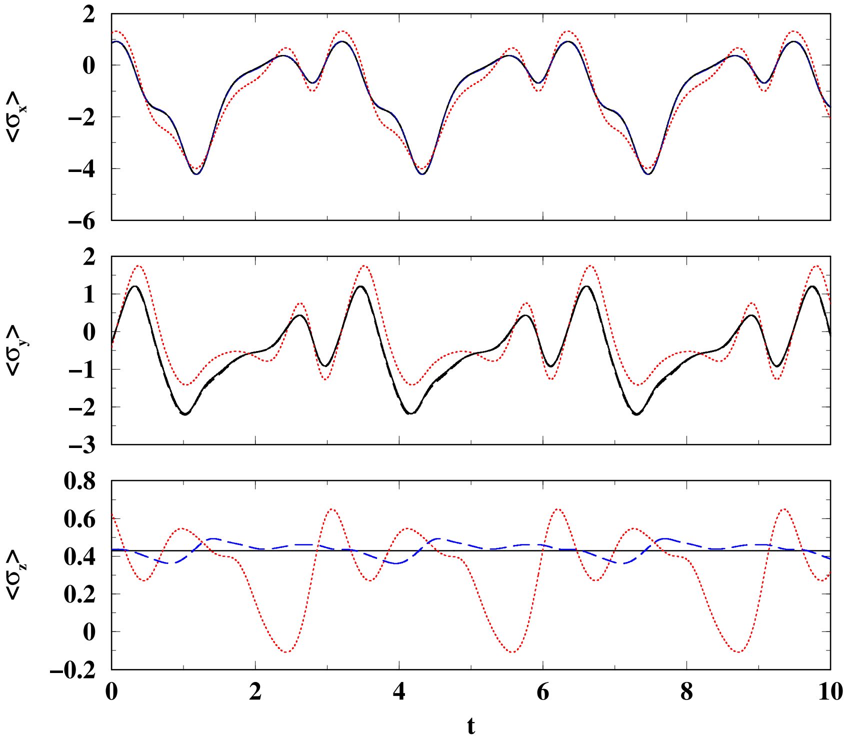

Fig. 5.13 Evolution of single mean values of $Tr_S(\rho_s(z_0'^* z_0' z_0^* z_0|t)\sigma_i$, with $i = \{x, y, z\}$ and normaliced initial condition $\rho_s(z_0'^* z_0' z_0^* z_0|0) = Tr_B\left(|\psi_0\rangle|z_0\rangle\langle z_0'|\langle\psi_0|/\langle\psi_0|\langle z_0'|z_0\rangle|\psi_0\rangle\right) = |\psi_0\rangle\langle\psi_0|/\langle\psi_0|\psi_0\rangle$. We have taken initial value already normalized $|\psi_0\rangle = \frac{(1+2i)|-\rangle+(1+i)|+\rangle}{\sqrt{7}}$. The average of equation (5.94) is numerically computed using the evolution (5.61) for an ensemble of 100 trajectories (dotted line) and 10^3 (long dashed line). The last result is practically equal to that of the solutions (5.108) and (5.109) obtained analytically (solid line).

procedure consists in plotting $C(m)$ with a high number of oscillators, and then sample it with $m = 6$ values of frequency. By doing this, the 6 frequencies of oscillators entering in the sum (5.112) will correspond to some of the most representative values of the coefficients. The comparison between (5.111) and the approximate correlation for 6 oscillators is shown in Figure 5.14.

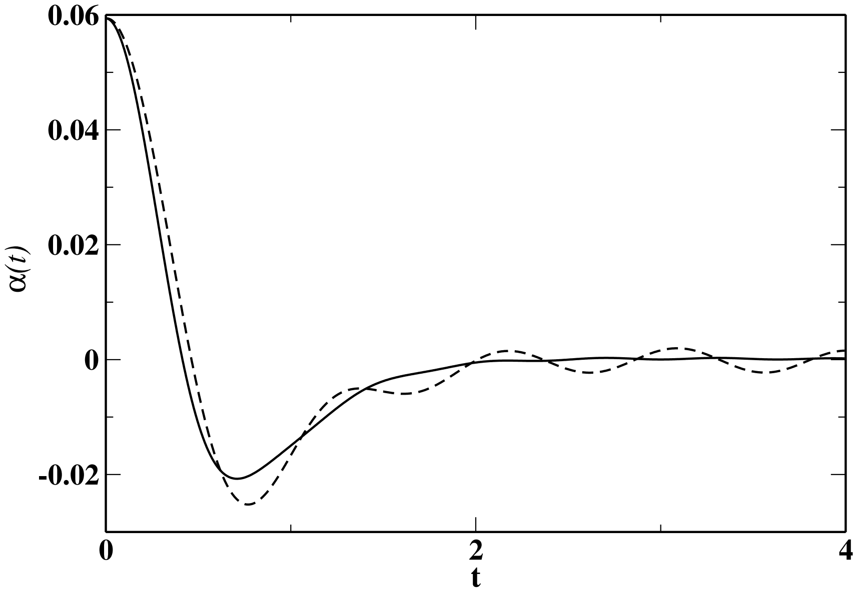

Fig. 5.14 Thermal correlation function $\alpha(t)$, given as (5.111) with $\beta = 10$ (solid line), compared to its Taylor expansion α^{appx} given as (5.112) with only $m = 6$ oscillators (long-dashed line). Despite the fact that the number of oscillators is very short, the approximation is quite good. This is due to the fact that the frequencies of those oscillators have been chosen between the most significant ones of the function $C(m)$.

For the thermal correlation function, we show in Figure (5.15) the evolution of $Tr_S(\rho_s(z_0'^* z_0' z_0^* z_0|t)\sigma_i)$, with $i = \{x, y, z\}$. It can be observed how the average of equation (5.94), which is numerically computed using the evolution (5.61), approaches to the result of (5.101) when a large enough ensemble of trajectories is used. Again, this is a numerical verification of the averages of the variable z_t that has been performed analytically by using a perturbative expansion of the propagators.

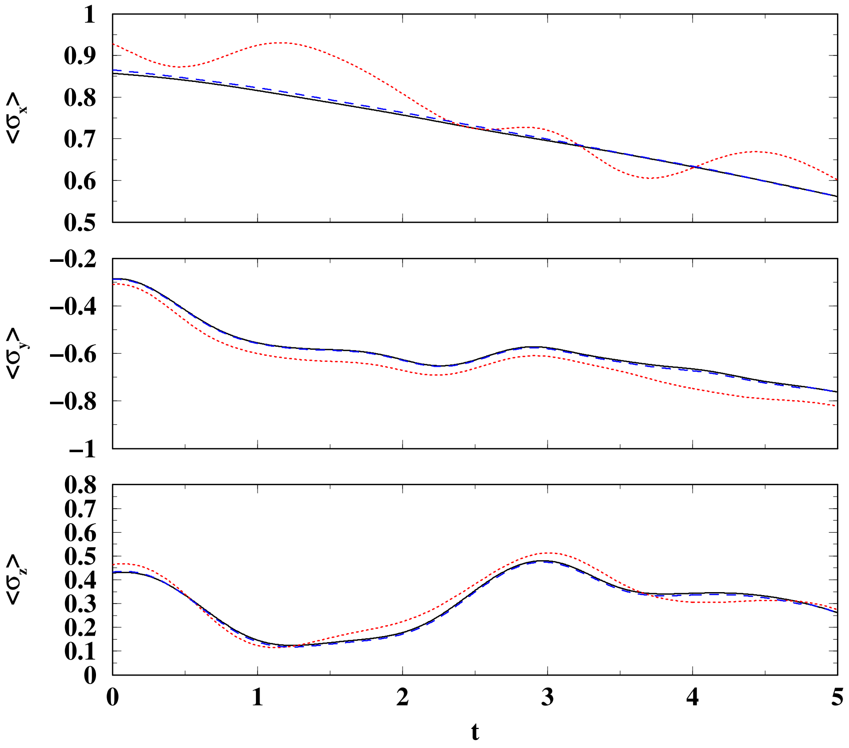

Fig. 5.15 Evolution of $Tr_S(\rho_s(z_0'^* z_0' z_0^* z_0|t)\sigma_i)$, with $i = \{x, y, z\}$ and normaliced initial condition $\rho_s(z_0'^* z_0' z_0^* z_0|0) = |\psi_0\rangle\langle\psi_0|/\langle\psi_0|\psi_0\rangle$. We have taken the value $|\psi_0\rangle = \frac{(1+2i)|-\rangle+(1+i)|+\rangle}{\sqrt{7}}$. The average of equation (5.94) is numerically computed using the evolution (5.61) for an ensemble of 14×10^3 trajectories (dotted line) and 18×10^6 (long dashed line). The latter result is practically equal to that of the general condition perturbative master equation (5.101) (solid line). The correlation function is obtained from the model (5.110) with 6 oscillators in the Fourier expansion (5.112), coupling parameter $g = 0.1$ and rotating frequency $\omega_S = 0.1$.

6

Conclusions of this part

We now briefly review the conclusions of this part of the thesis.

In Chapter (4) there was a brief introduction of Markovian and non-Markovian master and SSE. Although the results of this chapter are not original, they serve as a framework to contextualize the particular equations which are used in this work.

In Chapter (5) we presented some original results, which can be summarized as follows.

- In Section (5.1) different models of SSE are studied.
    - First, we compared two different stochastic linear equations, the convolutionless equation (5.21) [40, 39] and the convoluted equation (5.31) [35], showing that they are equivalent up to second order in the perturbation parameter. We have verified their equivalence numerically for a spin-boson system with a Hermitian coupling operator σ_x.
    - Second, we focused on the problem of sampling of SSE. When considering the effects of the interaction with the QOS in the probability distribution of the bath, the linear equation (5.21) gives rise to a second type of stochastic equation, which is non-linear with the wave function $|\psi_t(z^*)\rangle$, and which may evolve non-normalized states (in the case of equation (5.50)) or normalized states, in the case of equation (5.52) [40, 41]. Since they take into account the evolution of the environmental state distribution, non-linear equations are supposed to improve the sampling with respect to the linear ones. For the spin-boson model, the linear and the two non-linear equations have been studied for high and low temperatures, showing how the temperature is a very important parameter to decide whether it is necessary to use a non-linear equation. In non-linear equations, the effects of having a dynamical distribution are reflected in the use of a shifted noise $\tilde{z}_t$, instead of the original one.

      In the high temperature regime, the shifted noise $\tilde{z}_t$ becomes very different from the z_t that drives the linear equation, and the improvement in the sampling of non-linear equations is significant. The physical reason is that only for high temperatures the environmental distribution (Husimi) function $Q_t(z, z^*)$ may evolve considerably throughout the phase space. In such a case, non-linear equations lead to a much more efficient sampling than linear ones. At low temperatures, however, we show that the noise probability distribution does not evolve significantly and the shifted noise remains approximately equal to the non-shifted noise which drives the linear equation. As a consequence, the improvement in the sampling provided by non-linear equations is not very appreciable, and the best choice in this case is the simpler linear equation.

It is also interesting to point out that the non-linear equation that evolves normalized states (5.52), does not present a further improvement in the sampling (at least in the spin-boson model) in comparison with the non-linear equation (5.50) which still evolves non-normalized states,with the need, however, to keep track of the norm. While mathematically, both equations should give identical results, we here see that even in practical applications, there is no difference in the quality or efficiency of the results obtained from these two nonlinear equations, at least for the particular model studied.

- In Section (5.2) of the chapter, we have used the reduced propagators as a tool to derive different master equations by performing analytically the sum over the different initial and final states of the environment. This methodology can be found in the literature when such initial state is the vacuum. However, we have extended it to treat a new situation in which the environment and the system are initially correlated, generating a new master equation which depends on the environmental initial state. The extension of the methodology consists basically in a generalization of the Novikov theorem, on which is based the analytical average of the initial and final states. The generalization is needed in order to perform averages over reduced propagators in which the initial state is not the vacuum, and is explained in Appendix (I) and (J). In addition, we have considered the case in which system and environment are initially decorrelated, but the last one is in a thermal state. By using the general Novikov theorem and reduced propagators, it is obtained ithe same master equation for non-zero temperature already derived in the literature, which verifies the validity of our method.

Part III

MULTIPLE-TIME CORRELATION FUNCTIONS

7

Introduction and motivation

There are situations in which the expectation values of system observables are not enough to describe the essential features of the physical behavior of the system dynamics. Simple examples are found in statistical physics and spectroscopy, where the response of a system to an external electromagnetic field is studied. Particularly, in quantum optics, two-time correlation functions of the electromagnetic field emitted by an atom are useful in the study of the atomic spectroscopic properties. As a second example, the two-time correlations of the number of emitted photons, permit the description of a purely quantum mechanical effect, the photon anti-bunching. We illustrate this in the following section, where we also discuss the relation between the correlation of field operators and the correlation of system operators.

7.1 CORRELATIONS OF THE FIELD

Let us illustrate two examples of correlations in quantum optics. We start by studying the atomic emission spectra, which is related with two-time correlation of the field intensity. As a second example, we discuss the two-time correlations of the number of emitted photons, as well as their relation with the photon antibunching effect.

7.1.1 Atomic emission spectrum

Consider a rather idealized experimental set up for measuring the output spectrum of a quantum mechanical system, in our case, a set of two level atom linearly coupled with a radiation field. As explained in Chapter (1), the Hamiltonian of the emitting atom (with levels $|1\rangle$ and $|2\rangle$) is given by

$$H_S = -\frac{\omega_{12}}{2}(\sigma_{22} - \sigma_{11}) = \frac{\omega_{12}}{2}\sigma_z, \tag{7.1}$$

and the total Hamiltonian of emitting atom and radiation field is described by a Hamiltonian H_R, given by $H_R = H_S + H_B + \sum_\lambda g_\lambda (L^\dagger a_\lambda + a_\lambda^\dagger L)$. In order to detect the emitted radiation, suppose we have a detecting atom with Hamiltonian $H_{\mathcal{D}} = \Omega\sigma_z/2$, where Ω is its rotating frequency. The Hamiltonian of the total system (detector atom, emitting atom and radiation field) reads as follows,

$$H = H_{\mathcal{D}} + H_R + W. \tag{7.2}$$

Here the coupling between the detecting atom $H_{\mathcal{D}}$ with H_B is dipolar and given by a Hamiltonian W, which in interaction image with respect to the detector is given by

$$\tilde{W}(t) = \left[\sigma_{21}\mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(+)}(\mathbf{r}, t)e^{i\Omega t} + \sigma_{12}\mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(-)}(\mathbf{r}, t)e^{-i\Omega t}\right], \tag{7.3}$$

where we have considered $d_{21}^{\mathcal{D}}\hat{\mathbf{d}}^{\mathcal{D}} = d_{12}^{\mathcal{D}}\hat{\mathbf{d}}^{\mathcal{D}} = \langle 1 \mid \mathbf{D} \mid 2\rangle = \mathbf{d}^{\mathcal{D}}$. The superindex $\mathcal{D}$ reminds that these are the components of the detector's dipole. It is important to note here that the field operators $\mathbf{E}^{(+)}$ and $\mathbf{E}^{(-)}$, correspond to the radiative atoms and the radiation field with H_R. The positive part of the field situated in $(\mathbf{r})$ is defined in Chapter (1) as [1]

$$\mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t) = \sum_{\lambda} \epsilon_{\lambda} A_{\lambda}(\mathbf{r}) a_{\lambda}(\mathbf{r}_0, t)\mathbf{e}_{\lambda} \tag{7.4}$$

and $\mathbf{E}^{(-)}(\mathbf{r}, \mathbf{r}_0, t) = [\mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t)]^{\dagger}$ [50]. In the last expression (and from now on) we have added explicitly the dependency on the position $\mathbf{r}_0$ of the source dipole that originates the field. The quantity $\epsilon_{\lambda} = \sqrt{\frac{\omega_{\lambda}}{2\epsilon_0}}$, with υ the quantization volume. In terms of the coupling strengths we find that $g_{\lambda} \equiv g_{\lambda}(\mathbf{r}) = \epsilon_{\lambda} A_{\lambda}(\mathbf{r})\mathbf{d} \cdot \mathbf{e}_{\lambda}$.

As a condition, the time of observation T is much bigger that the inverse of the natural width Γ of the detecting atom excited level. In addition, the Rabi frequency of the emitting atom has to be bigger than the inverse of T. With this set up, the idea is to calculate the spectral distribution of the fluorescence light, $P(\Omega, T)$. This is defined as the probability of excitation of the detecting atom at the time of observation T, i.e.

$$P(\Omega, T) = Tr_{R,\mathcal{D}}\left(\mid 2\rangle\langle 2 \mid \rho(T)\right), \tag{7.5}$$

where $\rho(T)$ is the density matrix of the total system at time T. In interaction representation, this density matrix is,

$$\rho(T) = \rho(0) - i\int_0^T \left[\tilde{W}(t), \rho(0)\right] - \int_0^T dt \int_0^t dt' \left[\tilde{W}(t), \left[\tilde{W}(t'), \rho(0)\right]\right], \tag{7.6}$$

for an expansion in which $\rho(T) \approx \rho(0)$. Replacing (7.6) in (7.5), we get the following expression for $P(\Omega, T)$,

$$\begin{aligned} P(\Omega, T) = Tr_R \Bigg(& \int_0^T dt \int_0^t dt' e^{i\Omega(t-t')}\mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t)\rho_R \mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(-)}(\mathbf{r}, \mathbf{r}_0, t') \\ + & \int_0^T dt \int_0^t dt' e^{i\Omega(t'-t)}\mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t')\rho_R \mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(-)}(\mathbf{r}, \mathbf{r}_0, t)\Bigg). \end{aligned} \tag{7.7}$$

---

[1] We remind here that only in Chapter (1) and Appendix (A) of this work we use $\hbar \neq 1$. The reason is that they introduce the standard models for the system under study. We here follow the convention $\hbar = 1$ followed for simplicity in the rest of the work.

If we now change t into t', and t' into t in the second integral,

$$P(\Omega,T) = Tr_R\left(\int_0^T dt \int_0^t dt' e^{i\Omega(t-t')}\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},\mathbf{r}_0,t)\rho_R\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},\mathbf{r}_0,t')\right.$$
$$\left.+\quad \int_0^T dt' \int_0^{t'} dt e^{i\Omega(t-t')}\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},\mathbf{r}_0,t)\rho_R\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},\mathbf{r}_0,t')\right), \tag{7.8}$$

both integrands becomes the same. On the other hand, the regions of integration are the complementary parts of a square of side T (see Fig. (7.1)), so that the last expression can be written as

$$P(\Omega,T) = \int_0^T dt \int_0^T dt' e^{i\Omega(t-t')} g^{(1)}(\mathbf{r},\mathbf{r}_0;t,t'), \tag{7.9}$$

where the average $\langle\cdots\rangle = Tr_R\left(\rho_R\cdots\right)$, and we have defined

$$g^{(1)}(\mathbf{r},\mathbf{r}_0;t,t') = \langle\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},\mathbf{r}_0,t)\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},\mathbf{r}_0,t')\rangle, \tag{7.10}$$

as the first order correlation of the projection of the emitted field in the direction of the dipole.

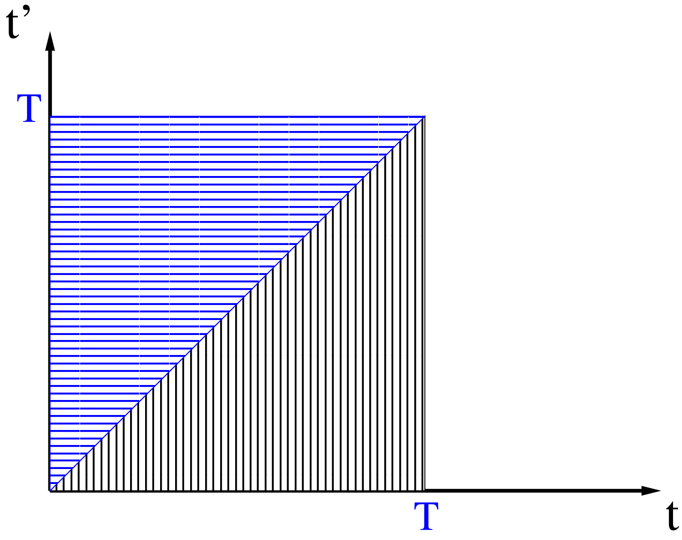

Fig. 7.1 The figure displays the regions of integration of equation (7.8).

In order to express the last equation in terms of observables of the emitting atoms, it is necessary to express the field operator, which is defined in (7.4) in terms of the atomic dipolar momentum. We insert in (7.4) the solution of the Heisenberg equation for $a_\lambda(\mathbf{r}_0,t)$ with the total Hamiltonian (7.2) , i.e. $da_\lambda(\mathbf{r}_0,t)/dt = -i[H_B, a_\lambda(\mathbf{r}_0,t)]$,

$$a_n(\mathbf{r}_0,t) = a_\lambda(\mathbf{r}_0,0)e^{-i\omega_\lambda\tau} - i\int_0^t d\tau g_\lambda L(t')e^{-i\omega_\lambda(t-\tau)} \tag{7.11}$$

a result which has been already obtained in (2.38). Here, the coupling constant between emitting atoms and surrounding field is $g_\lambda \equiv g_\lambda(\mathbf{r}_0) = \epsilon_\lambda A_\lambda(\mathbf{r}_0)\mathbf{d}\cdot\mathbf{e}_\lambda$. After this replacement, the component of $\mathbf{E}^{(+)}$ in the direction and position of the detector is

$$\mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t) = -i \sum_{\lambda} g_{\lambda} g_{\lambda}^{\mathcal{D}} \int_0^t d\tau L(\tau) e^{-i\omega_{\lambda}(t-\tau)}, \tag{7.12}$$

where we have defined $g_{\lambda}^{\mathcal{D}} \equiv g_{\lambda}^{\mathcal{D}}(\mathbf{r}) = \epsilon_{\lambda} A_{\lambda}(\mathbf{r}) \mathbf{d}^{\mathcal{D}} \cdot \mathbf{e}_{\lambda}$ as the coupling constant of the detector with the emitted field. In expression (7.12) we only keep the part of the field corresponding to the radiated field from the dipole (also "source field"). The other part, corresponding to the quantum vacuum field

$$\mathbf{E}_0^{(+)}(\mathbf{r}, \mathbf{r}_0, t) = \sum_{\lambda} \epsilon_{\lambda} A_{\lambda}(\mathbf{r}) a_{\lambda}(\mathbf{r}_0, 0) e^{-i\omega_{\lambda} t} \mathbf{e}_{\lambda}, \tag{7.13}$$

does not contribute to photodetection signals, since provided that the field is in the vacuum state $|0\rangle$,

$$\begin{aligned} \langle 0| \left(\mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}_0^{(-)}(\mathbf{r}, \mathbf{r}_0, \tau) \right) &= 0 \\ \left(\mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}_0^{(+)}(\mathbf{r}, \mathbf{r}_0, 0) \right) |0\rangle &= 0 \end{aligned} \tag{7.14}$$

in (7.10). We now introduce a distribution function $\rho(\mathbf{r}_0)$, which describes the density of radiating atoms at a given positions of the crystal. Assuming that the atomic distribution is the same for each Wigner Seitz cell (WSC) of the crystal [106], we perform an average over the atomic distribution within the crystal, obtaining the following expression for the positive part of the radiation field,

$$\langle \mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t) \rangle_{\mathbf{r}_0} = \frac{1}{N_e} \int_{WSC} d\mathbf{r}_0 \rho(\mathbf{r}_0) \mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t) \tag{7.15}$$

where $N_e = \int_{WSC} d\mathbf{r}_0 \rho(\mathbf{r}_0)$ is the number of active atoms in a cell. Considering one single atom at position $\mathbf{r}_a$ in each cell, such that $\rho(\mathbf{r}_0) = \delta(\mathbf{r}_0 - \mathbf{r}_a)$ and $N_e = 1$. Then we have

$$\langle \hat{\mathbf{d}}_D \cdot \mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_0, t) \rangle_{\mathbf{r}_0} = -i \int_0^t d\tau \mathcal{S}(\mathbf{r}, \mathbf{r}_a, t, \tau) L(\tau) \tag{7.16}$$

with the $\mathcal{S}(\mathbf{r}, \mathbf{r}_a, t, \tau) = \sum_{\lambda} g_{\lambda}^{\mathcal{D}} g_{\lambda} e^{-i\omega_{\lambda}(t-\tau)}$, with $g_{\lambda} \equiv g_{\lambda}(\mathbf{r}_a)$. Replacing (7.16) in the integrand of (7.9), we get

$$\begin{aligned} g^{(1)}(\mathbf{r}, \mathbf{r}_a, t, t') &= \langle g^{(1)}(\mathbf{r}, \mathbf{r}_0, t, t') \rangle_{\mathbf{r}_0} \\ &= \left\langle \left(\langle \mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(-)}(\mathbf{r}, \mathbf{r}_a, t) \rangle_{\mathbf{r}_0} \right) \left(\langle \mathbf{d}^{\mathcal{D}} \cdot \mathbf{E}^{(+)}(\mathbf{r}, \mathbf{r}_a, t') \rangle_{\mathbf{r}_0} \right) \right\rangle \\ &= \int_0^t d\tau \int_0^{t'} d\tau' \mathcal{S}^*(\mathbf{r}, \mathbf{r}_a, t, \tau) \mathcal{S}(\mathbf{r}, \mathbf{r}_a, t', \tau') \langle L^{\dagger}(\tau) L(\tau') \rangle \end{aligned} \tag{7.17}$$

Following (7.9) the spectra has the following form,

$$\begin{aligned} P(\Omega, T) &= \int_0^T dt \int_0^T dt' e^{i\Omega(t-t')} g^{(1)}(\mathbf{r}, \mathbf{r}_a, t, t') \\ &= \int_0^T dt \int_0^T dt' e^{i\Omega(t-t')} \left\{ \int_0^t d\tau \int_0^{t'} d\tau' \mathcal{S}^*(\mathbf{r}, \mathbf{r}_a, t, \tau) \mathcal{S}(\mathbf{r}, \mathbf{r}_a, t', \tau') \right. \\ &\quad \left. \times \langle L^{\dagger}(\tau) L(\tau') \rangle \right\}. \end{aligned} \tag{7.18}$$

When there is no spatial dependency of the functions $\mathcal{S}^*(\mathbf{r},\mathbf{r}_a,t,\tau)$, then they are the usual correlation functions $\alpha(t-\tau)$. In that case, we can write (7.18) as

$$P(\Omega,T) = \int_0^T dt \int_0^T dt' e^{i\Omega(t-t')} \left\{ \int_0^t d\tau \int_0^{t'} d\tau' \alpha^*(t-\tau)\alpha(t'-\tau')\langle L^\dagger(\tau)L(\tau')\rangle \right\}. \quad (7.19)$$

In addition, in the Markov case, such correlation is a delta function, $\alpha(t-\tau) = \Gamma\delta(t-\tau)$, and the last formula is just

$$P(\Omega,T) = \Gamma^2 \int_0^T dt \int_0^T dt' e^{i\Omega(t-t')}\langle L^\dagger(t)L(t')\rangle. \quad (7.20)$$

In the case of fluorescence, this expression has to be averaged in time, in such a way that in the long time limit, and provided that the field operators are correlated only over a short period of time, the power spectra is defined as [43],

$$P(\Omega) = lim_{T\to\infty}\frac{1}{T}P(\Omega,T) = \Gamma^2 Real\left[\int_0^\infty d\tau e^{i\Omega\tau}\langle L^\dagger(0)L(\tau)\rangle\right] \quad (7.21)$$

The system correlations $\langle L^\dagger(0)L(\tau)\rangle$ can be computed with the Quantum Regression Theorem. In the non-Markovian case, we cannot assume that the correlation function is a delta, and it is necessary to use the original formula, (7.19). In addition, as we will show in this part of the thesis, for non-Markovian interactions that an alternative theory to the QRT is needed to compute the system correlation functions. The derivation of such a theory, which we also present here, is therefore necessary for the description of non-Markovian emission spectra.

7.1.2 Joint emission probability and photon antibunching.

Just in the same way as in the former section, the probability $P(t,t')$ of detecting a photon at time t and another one at a later time $t' = t+\tau$ is related to higher order correlation functions of the electric field,

$$\begin{aligned} g^{(2)}(t,t') &= \langle \mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},t)\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},t')\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},t')\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},t)\rangle \\ &= \int_0^t d\tau \int_0^{t'} d\tau' \mathcal{S}^*(\mathbf{r},\mathbf{r}_a,t,\tau)\mathcal{S}^*(\mathbf{r},\mathbf{r}_a,t',\tau') \\ &\quad \times \int_0^t ds \int_0^{t'} ds' \mathcal{S}(\mathbf{r},\mathbf{r}_a,t,s)\mathcal{S}(\mathbf{r},\mathbf{r}_a,t',s')\langle L^\dagger(\tau)L^\dagger(\tau')L(s')L(s)\rangle. \end{aligned} \quad (7.22)$$

Here, a four-time correlation function $\langle L^\dagger(\tau)L^\dagger(\tau')L(s')L(s)\rangle$ of the system coupling operator is needed. The former correlation can normalised as

$$\tilde{g}^{(2)}(t,t') = \frac{\langle \mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},t)\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},t')\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},t')\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},t)\rangle}{\langle \mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},t)\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},t)\rangle\langle \mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(-)}(\mathbf{r},t')\mathbf{d}^{\mathcal{D}}\cdot\mathbf{E}^{(+)}(\mathbf{r},t')\rangle}. \quad (7.23)$$

When the radiation field consists in a single mode, then most factors cancel in the mode expansions for $\mathbf{E}^{(-)}$ and $\mathbf{E}^{(+)}$, and the former expression is just the time ordered average of the correlation of the photon number $n = a^\dagger a$,

$$\tilde{g}^{(2)}(\tau) = \frac{\langle : n(t)n(t+\tau) :\rangle}{\langle n(t)\rangle^2}, \quad (7.24)$$

where $: * :$ represents the time-ordered sequence of the operators inside. The time dependency is over the total system Hamiltonian. As noted in the introduction, the measurement of $\tilde{g}^{(2)}(\tau)$ permits the description of the so-called photon antibunching. This effect, first described by Glauber in [48], consists in an initial positive slope of the two-time correlation function of number of emitted photons. In 1975, Carmichael and Walls [107] predicted that photon antibunching can be generated in resonance fluorescence of a two-level atom, being experimentally observed in 1977 by Kimble et al [108]. While for the light emitted by a thermal source $\tilde{g}^{(2)}(0) = 2$, indicating the tendency of photons to be emitted in *bunches* (photon bunching), in resonance fluorescence we find $\tilde{g}^{(2)}(0) = 0$, indicating the tendency of the photons to be emitted in a separated way, or an anti-bunching effect. This last result is due to the thermal nature of the light emitted by resonance fluorescence. The detection of the first photon prepares the atom in the ground state. Since any subsequent emission must begin with an excited atom, a delay corresponding to the time taken for the atom to be re-excited is naturally expected. Antibuching is therefore a purely quantum effect, not predicted by classical theory. Additionally, it is only expected for the emission of a single atom, since the time-delay of successive emissions is not appreciable when having a large number of independent emitting atoms, as occurs with thermal light.

Further discussions about photon bunching and antibunching can be found in [21, 43, 53] for Markovian type of interactions.

Before starting with our theory, let us present in the next section a brief discussion about the Markovian theory of quantum fluctuations.

7.2 MARKOVIAN INTERACTIONS: THE QUANTUM REGRESSION THEOREM

In the Markov case, it is possible to derive a formula which permits the evaluation of two-time correlations (and even N-time correlations) using the master equation for the reduced density operator. This result, which was first obtained by Lax [18, 19], receives the name of Quantum Regression Theorem [2]. It should be noted here that there is a classical hypothesis by Onsager [17] which leads to the same formula as the QRT for two-time correlations. However, as noted by Carmichael in [53], the difference between both formulas is that Onsager's concerns fluctuations about the equilibrium, while the Lax formula is valid for calculating two time correlations even in the non-equilibrium case. We here follow the derivation of the Quantum Regression Theorem presented in [51]. Analogous derivations might be found in the original paper of Lax, and also in several books of Quantum Optics, for instance [43, 50, 53].

Suppose that we have a certain set of system operators A_i, and that for some initial value of the density operator ρ_s, the evolution of their quantum mean values is given by the master equation,

$$\frac{d}{dt}\langle A_i(t)\rangle = \sum_j G_{ij}(t)\langle A_j(t)\rangle, \tag{7.25}$$

where $\langle A_i(t)\rangle = Tr_S\left(\rho_S(t)A_i\right)$. Then, we can assert that

$$\frac{d}{d\tau}\langle A_i(t_1)A_l(t_2)\rangle = \sum_j G_{ij}(t_1)\langle A_j(t_1)A_l(t_2)\rangle. \tag{7.26}$$

Let us consider the two time correlation function of operators $A_1 = A$ and $A_2 = B$ [51],

$$\langle A(t_1)B(t_2)\rangle \quad = \quad Tr_S Tr_B\Big(\mathcal{U}^{-1}(t_2,0)\mathcal{U}^{-1}(t_1,t_2)A\mathcal{U}(t_1,t_2)$$

---

[2] Although as noted by Carmichael in [53] it would be more appropriate to use the word "formula" instead of "theorem".

$$\times\mathcal{U}(t_2,0)\mathcal{U}^{-1}(t_2,0)B\mathcal{U}(t_2,0)\rho_{tot}(0)\Big), \tag{7.27}$$

where the unitary evolution operator from t_2 to $t_1 = t_2 + \tau$, which is assumed to be in interaction picture, is

$$\mathcal{U}(t_1,t_2) = e^{iH_0 t_1} e^{-iH_{tot}(t_1-t_2)} e^{-iH_0 t_2}. \tag{7.28}$$

Considering the unitarity of the evolution operators $\mathcal{U}(t,0)\mathcal{U}^{-1}(t,0) = 1$ and the cyclic property of the trace, we can write (7.27) as,

$$\langle A(t_1)B(t_2)\rangle = Tr_A\left(ATr_B\left\{\mathcal{U}(t_1,t_2)B\rho_{tot}(t_2)\mathcal{U}^{-1}(t_1,t_2)\right\}\right), \tag{7.29}$$

where $\rho_{tot}(t_2) = \mathcal{U}(t_2,0)\rho_{tot}(0)\mathcal{U}^{-1}(t_2,0)$. Let us now consider the evolution equation of the term inside the brackets of the environmental trace

$$\xi(t_1,t_2) = \mathcal{U}(t_1,t_2)B\rho_{tot}(t_2)\mathcal{U}^{-1}(t_1,t_2), \tag{7.30}$$

with respect to t_1 and in interaction picture,

$$\frac{d\xi(t_1,t_2)}{dt_1} = \frac{1}{i}[V_{t_1}H_I, \xi(t_1,t_2)]. \tag{7.31}$$

The form of this equation is identical to the von-Neumann equation for $\rho_{tot}(t_2)$ in interaction picture, (4.4). Hence, in order to obtain a closed evolution equation for $Tr_B\left(\xi(t_1,t_2)\right)$, we can follow the same procedure we used in Section (4.1.2.2) for obtaining the master equation up to second order in g. In that way, performing a perturbative expansion of (7.31), and then deriving the result, we get

$$\frac{d\xi(t_1,t_2)}{dt_1} = -i[V_{t_1}H_I, \xi(t_2,t_2)] - \int_{t_2}^{t_1} d\tau\, [V_{t_1}H_I, [V_{t_1-\tau}H_I, \xi(t_2,t_2)]], \tag{7.32}$$

with

$$\xi(t_2,t_2) = B\rho_{tot}(t_2). \tag{7.33}$$

We can now proceed to trace out the bath degrees of freedom, so that the final equation for $Tr_B\left(\xi(t_1,t_2)\right) = \xi^S(t_1,t_2)$ can be written in a similar way as (4.9),

$$\frac{d\xi^S(t_1,t)}{dt_1} = -\int_t^{t_1} d\tau Tr_B\Big([V_{t_1}H_I, [V_{t_1-\tau}H_I, \xi^B(t,t)]]\Big)\xi^S(t,t), \tag{7.34}$$

where we have assumed an initially decorrelated state $\xi(t_2,t_2) = \xi^B(t_2,t_2)\otimes\xi^S(t_2,t_2)$, which since the definition (7.33), is equivalent to assuming the Born approximation. Assuming that the $\xi^S(t_1,t_2) = \xi^S(t_2,t_2) + \mathcal{O}(g)$, we can approximate the last equation, up to second order as

$$\frac{d\xi^S(t_1,t_2)}{dt_1} = -\int_{t_2}^{t_1} d\tau Tr_B\Big([V_{t_1}H_I, [V_{t_1-\tau}H_I, \xi^B(t_2,t_2)]]\Big)\xi^S(t_1,t_2), \tag{7.35}$$

which is **not** equal to the master equation (4.11), because of the limits of integration. Only in the Markov case, the former equation in which the integral disappears and the equation becomes local in time, the evolution equation of $\xi^S(t_1,t_2)$ becomes equal to the Linbland master equation (4.3),

$$\frac{d\xi^S(t_1,t_2)}{dt_2} = -i[H_S, \xi^S(t_1,t_2)] + \frac{1}{2}([L\xi^S(t_1,t_2), L^\dagger] + [L, \xi^S(t_1,t_2)L^\dagger]), \tag{7.36}$$

with initial condition $\xi^S(t_2,t_2) = Tr_B(B\rho_{tot}(t_2)) = B\rho_S(t_2)$. In this relation, one can easily observe that the evolution equation in t_1 has the same form as an ordinary master equation, but considering as initial condition $B\rho(t_2)$. This procedure can be repeated to show that, in general, N-time correlation functions are computed by considering the $N-1$-time correlations as initial condition, and using the evolution equation of 1-time correlations, namely the Markovian master equation.

The last derivation can be mathematically expressed in terms of the so-called evolution super-operators, $\mathcal{Z}(t_1,t_2)$, which define the following mapping over the operator $\xi^S(t_1,t_2)$ (see [38, 51] for further details),

$$\xi^S(t_1,t_2) = \mathcal{Z}(t_1,t_2)\xi^S(t_2,t_2). \tag{7.37}$$

The evolution equation of $\mathcal{Z}(t_1,t_2)$ has the same form as the evolution of $\xi^S(t_1,t_2)$ which, as derived above, turns out to be equal to the evolution for $\rho_s(t_1)$, but with a different initial condition. The important fact about evolution superoperators is that they have the semigroup property,

$$\mathcal{Z}(t_1,t_2)\mathcal{Z}(t_2,t_0) = \mathcal{Z}(t_1,t_0), \tag{7.38}$$

but only when they are Markovian, i.e. when the memory effects can be neglected in the system dynamics. In terms of $\mathcal{Z}(t_1,t_2)$, the two-time correlation (7.29) can be written as

$$\langle A(t_1)B(t_2)\rangle = Tr_A\left(A\mathcal{Z}(t_1,t_2)Tr_B\left(B\rho_{tot}(t_2)\right)\right). \tag{7.39}$$

In addition, the theory of stochastic Schrödinger equations, initially elaborated to compute the expectation values of system observables, has been extended by many groups [56, 58, 59] to calculate multiple-time correlation functions for the Markovian case. Such stochastic methods agree with the results expected from the QRT.

7.3 NON-MARKOVIAN INTERACTIONS

It is natural to develop a theory equivalent to that existing for Markovian interactions, in order to evaluate multiple-time correlation functions for systems with *non-Markovian* effects, such as atom lasers formed from Bose-Einstein condensates. Another interesting application of non-Markovian multiple-time correlation function is an atom immersed in the modified radiation field that exists in a Photonic crystal (PC) [109]. As will be later explained, in PCs the refraction index is periodic, which produces Bragg scattering of photons with wave lengths related with the periodicity of the lattice. As a consequence, those photonic modes do not appear within the crystal, and the dispersion relation of the electromagnetic field displays a band structure interrupted with gaps of forbidden frequencies. In such structured materials, within the edges of the bands, the correlation function of the electromagnetic field is highly non-Markovian. Therefore, the dynamics of an atom interacting with such radiation field, including its fluctuations is typically non-Markovian.

In this part of the thesis, we intend to complete the description of non-Markovian quantum open systems by generating a theory of MTCFs. To this purpose, we describe the dynamics of the QOS with the system *reduced propagator*. The reduced propagator was introduced in Chapter (2), where we also made a general description of how MTCFs can be written in terms of these. In the next section we summarize this discussion by considering particularly an initially decorrelated state between system and environment, $\rho_{tot} = |\psi_0\rangle\langle\psi_0| \otimes |0\rangle\langle 0|$, which is here chosen for deriving the dynamical equations. In Appendix (L) the dynamical equation for two-time correlation functions within a thermal environment is computed.

7.3.1 Multiple-time correlation functions from reduced propagators

We start as usual from the model Hamiltonian introduced in Chapter (1) to study the dynamics of $\mathcal{S}$ with Hamiltonian H_S, in interaction with $\mathcal{B}$

$$H_{tot} = H_S + L \sum_\lambda g_\lambda \left(a_\lambda^\dagger L + L^\dagger a_\lambda \right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda. \tag{7.40}$$

We are interested in the evaluation of *N-time correlation functions*. For a set of observables in Heisenberg representation, $\{A_1(t_1), \cdots, A_N(t_N)\} = \mathbf{A}(\mathbf{t})$, we defined them in Section (2.2) as

$$C_{A_1,A_2,\cdots,A_N}(t_1,t_2,\cdots,t_N|\Psi_0) = C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \langle\Psi_0|A_1(t_1)\cdots A_N(t_N)|\Psi_0\rangle, \tag{7.41}$$

with $t_1 > t_2 > \cdots > t_N$ and $\mathbf{t} = \{t_1, \cdots, t_N\}$. Particularly, we have chosen here the initial state of the full system as the tensor product of a system state $|\psi_0\rangle$ and the environment state $|z_0\rangle$, *i.e.* $|\Psi_0\rangle = |\psi_0\rangle|z_0\rangle$, as defined in Section (2.2.1).

In the partial interaction picture with respect to the environment, the N-time correlation function is defined as

$$C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \langle\Psi_0| \prod_{i=1}^{N} \mathcal{U}_I^{-1}(t_i,0) A_i \mathcal{U}_I(t_i,0)|\Psi_0\rangle, \tag{7.42}$$

It is important to stress that in this part of the thesis two different time dependencies for the system operators will often appear:

- A time dependency on the Hamiltonian of the $total$ system is denoted by $A_i(t_i) = \mathcal{U}_I^{-1}(t_i,0)A_i\mathcal{U}_I(t_i,0)$, where $\mathcal{U}_I$ is the evolution operator of the total system in the interaction picture,
$$\mathcal{U}_I(t_i t_{i+1}) = e^{iH_B t_i} e^{-iH_{tot}(t_i - t_{i+1})} e^{iH_B t_{i+1}}. \tag{7.43}$$
- A time dependency with the free Hamiltonian of the *systems* and *environment* H_0 is denoted by $V_{t_i} A_i = \exp\{i\mathcal{L}_S t_i\} L = \exp(iH_0 t_i) A_i \exp(-iH_0 t_i) = \exp(iH_S t_i) A_i \exp(-iH_S t_i)$, where therefore $V_{t_i} = \exp\{i\mathcal{L}_S t_i\}$ is the free system Liouville operator, acting in the two sides of the inmediatly contiguous system operator.

In the Bargmann basis for the environment, $|z_1, z_2, \cdots, z_\lambda, \cdots\rangle = |z\rangle$, the resolution of the identity is given by [43, 48] $\mathit{1} = \int d\mu(z)|z\rangle\langle z|$, with $d\mu(z)$ defined in (2.5). If we introduce N identity operators in (7.42), the correlation function is given by

$$C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \int \left(\prod_{i=1}^{N} d\mu(z_i) \right) \langle\psi_0|G^\dagger(z_0^* z_1|t_0 t_1) \prod_{i=1}^{N} A_i G(z_i^* z_{i+1}|t_i t_{i+1})|\psi_0\rangle, \tag{7.44}$$

with the definitions $t_0 = 0$, $t_{N+1} = 0$, $z_{N+1} = z_0$, in terms of the reduced propagators $G(z_i^* z_{i+1}|t_i t_{i+1}) = \langle z_i|\mathcal{U}_I(t_i, t_{i+1})|z_{i+1}\rangle$ introduced in Chapter (2). With the expression (7.44), the evolution equation of multiple-time correlation functions is formally given by

$$\begin{aligned} \frac{dC_{\mathbf{A}}(\mathbf{t}|\Psi_0)}{dt_1} &= \int d\mu(z)\langle\psi_0|\frac{\partial G^\dagger(z_0^* z_1|t_0 t_1)}{\partial t_1} \prod_{i=1}^{N} A_i G(z_i^* z_{i+1}|t_i, t_{i+1})|\psi_0\rangle \\ &+ \int d\mu(z)\langle\psi_0|G^\dagger(z_0^* z_1|t_0 t_1) A_1 \frac{\partial G(z_1^* z_2|t_1, t_2)}{\partial t_1} \prod_{i=2}^{N} A_i G(z_i^* z_{i+1}|t_i, t_{i+1})|\psi_0\rangle, \end{aligned} \tag{7.45}$$

As noted before, we consider for simplicity the case in which the initial state of the bath is the vacuum, $z_0 = 0$. The evolution equations for two-time correlations with an initial condition for the environment different than the vacuum (particularly a thermal environment), will be derived in Appendix (L).

It is clear from (7.45) that once the evolution in time of the reduced propagator is solved, then the time-correlation function (7.44) can be obtained. Therefore, to proceed further we need to use the equation of motion of the reduced propagator $G(z_i^* z_{i+1}|t_i t_{i+1})$. This equation was derived in Chapter (2), in two different versions, an open equation in the total Hilbert space (equation (2.40)) ,

$$\begin{aligned} \frac{\partial G(z_i^* z_{i+1}|t_i t_{i+1})}{\partial t_i} &= \big(-iH_S + L z_{i,t_i}^* - L^\dagger z_{i+1,t_i} \big) G(z_i^* z_{i+1}|t_i t_{i+1}) \\ &- L^\dagger \int_{t_{i+1}}^{t_i} d\tau \alpha(t_i - \tau) \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle, \end{aligned} \tag{7.46}$$

where, as usual

$$z_{i,t} = i \sum_\lambda g_\lambda z_{i,\lambda} e^{i\omega_\lambda t}, \tag{7.47}$$

and,

$$\alpha(t-\tau) = \sum_\lambda g_\lambda^2 e^{-i\omega_\lambda (t-\tau)}, \tag{7.48}$$

and a closed equation in the Hilbert space of the system in which the matrix element in the last term was expressed as

$$\langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle = O(z_{i+1} z_i^*, t, \tau) G(z_i^* z_{i+1}|t_i t_{i+1}), \tag{7.49}$$

generally with the use of some approximation. In that case, the equation was expressed in terms of the reduced propagator as

$$\begin{aligned} \frac{\partial G(z_i^* z_{i+1}|t_i t_{i+1})}{\partial t_i} &= \big(-iH_S + L z_{i,t_i}^* - L^\dagger z_{i+1,t_i} \big) G(z_i^* z_{i+1}|t_i t_{i+1}) \\ &- L^\dagger \int_{t_{i+1}}^{t_i} d\tau \alpha(t_i - \tau) O(z_{i+1} z_i^*, t, \tau) G(z_i^* z_{i+1}|t_i t_{i+1}). \end{aligned} \tag{7.50}$$

The equations used in this chapter are linear, since the environment distribution function is considered constant during the interaction with the system. As already seen in Chapter (5), this is a good approximation for environments at low temperature. However, when the environment is at high temperatures, then its state distribution changes considerably due to the interaction [1].

In order to take this into account, the statistical distribution of the noise has to be considered in evolution, and this is precisely what non-linear equations do [40]. In Appendix (H.2), we present a non-linear equation for the propagator $G(z_i^* z_{i+1}|t_i t_{i+1})$ that has been derived following the same method used by Diósi, Gisin and Strunz in [40] to generate the non-linear equation for vacuum propagators $G(z_i^* 0|t_i 0)$. It is important to stress that the use of a non-linear equation instead of a linear one is only necessary to improve the sampling when the MTCFs are obtained numerically. It is evident that an analytical average (which does not depend on the sampling) over both non-linear and linear equations gives rise to the same MTCF equations.

The study of MTCF is divided in three chapters:

- Chapter (8): The open form of the reduced propagator (7.46) is used to derive a set of MTCF without the use of any approximation. This equations are ordered in a *hierarchy*, in such a way that N-time correlations depend on $N+1$-time correlations. The hierarchy represents a useful tool to derive the general equation for non-Markovian N-time correlations. This equation provides an excellent basis to compute N-time correlations once the appropriate approximations are made in order to destroy the dependency with higher order correlations [2]. Indeed, since the hierarchy is an open structure, its practical use is limited to those cases in which such dependency can be broken. This can be done within the weak coupling approximation, as discussed in Chapter (9).

- Chapter (9): We use a second order perturbative approximation with respect to the coupling constant, which destroys the dependency of N-time correlations with $N+1$ [4]. In this part we use the closed equation for the reduced propagator (7.50), with $O(z_{i+1}z_i^*, t, \tau) = V_{\tau-t}L + \mathcal{O}(g)$, to obtain an equation up to second order in g. Three methods are then proposed to compute MTCF: First, *stochastic sampling*, based on evolving the propagator by choosing random realizations of the variables z_i and z_{i+1}, and then performing numerically an average over different trajectories. Second *perturbative expansion*, in which MTCF are computed by inserting the perturbative expansion of the propagators into (7.45), and then performing analytically the Gaussian averages of the variables z_{i,t_i} and z_{i+1,t_i}. These first two methods are illustrated by computing two-time correlations. The third method consists in applying the perturbative hypothesis to the *hierarchy* of equations. As noted above, the hierarchy is broken: the dependency on higher order vanishes, and closed equations for N-time correlations are obtained. For two-time correlations, the equation is shown to be the same as the one obtained with the perturbative expansion. A three-time correlation is also obtained. The main advantage of using the second order perturbative hypothesis in the hierarchy of equations is that it permit us to obtain easily a general equation of non-Markovian MTCF.

Let us make a comment about the **time-ordering** of multiple-time correlation functions. In this part of the thesis, we start by deriving the evolution equation of multiple-time correlation functions $C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \langle A_1(t_1)\cdots A_N(t_N)\rangle$ with $\mathbf{t} \equiv t_N \leq \cdots \leq t_1$. Nevertheless, in Appendix (M) is shown how to derive a new type of correlations $C_{\mathbf{A}',\mathbf{A}}(\mathbf{t}', \mathbf{t}|\Psi_0) = \langle \Psi_0|A'_N(t'_N)\cdots A'_2(t'_2)A_1(t_1)\cdots A_N(t_N)|\Psi_0\rangle$, with the time ordering such that $t'_n \leq t'_{N-1} \leq \cdots \leq t'_2 \leq t_1$ and $t_n \leq t_{N-1} \leq \cdots \leq t_2 \leq t_1$. These $2N+1$-time correlation functions can correspond to a sequence of measurements performed over the system. On the other hand, formula (7.22) expresses in a clear way that correlations with these time orderings are not the only ones needed to describe the other quantities such as the joint emission probability of a photon $P(t', t)$. Nevertheless, we stress that although we only compute the evolution of $C_{\mathbf{A}}(\mathbf{t}|\Psi_0)$ and $C_{\mathbf{A}',\mathbf{A}}(\mathbf{t}', \mathbf{t}|\Psi_0)$ with the time-ordering described above, the methods derived in this thesis are useful *for any given time ordering for multiple-time correlation functions*.

8

Hierarchy of non-Markovian MTCF

We derive in this Chapter the **hierarchy** of equations that formally obey non-Markovian MTCFs, when no approximations are made. To this end, two different methods are used: the first, described in Section (8.1), is based on using system propagators, while the second, discussed in Section (8.2), relies on the use of the Heisenberg equation of system operators.

The hierarchy structure consists in the following: The evolution equation of one-time correlations (i.e. quantum mean values), depends on two-time correlations. Furthermore, the evolution equation of two time correlations depends on three-time correlations. The same happens with the evolution equation for three time correlations, which also shows a dependency on fourth order correlations. In summary, the evolution of non-Markovian N-time correlations of system operators, when no approximations are made, depends on the $N+1$-time correlations.

The hierarchy only occurs in non-Markovian interactions, since it vanishes when the bath correlation function $\alpha(t)$ is chosen Markovian, i.e. $\alpha(t) = \Gamma\delta(t)$. In the non-Markovian case, in order to make practical use of the MTCF equations, it is necessary to break up the hierarchy and eliminate the dependency on higher order correlation functions by using some approximations. This is done in the next chapter by considering a second order perturbative approximation.

8.1 METHOD I: MTCF IN THE SCHRÖDINGER FORMALISM

8.1.1 Evolution equation of one-time correlations

We present in this section the evolution of the quantum mean value of a system operator A. Following the general form (7.45), it is given by

$$\frac{dC_A(t|\Psi_0)}{dt} = \mathcal{M}_1\left[\langle\psi_0|\frac{\partial G^\dagger(0z_1|0t_1)}{\partial t_1}AG(z_1^*0|t_10)|\psi_0\rangle\right]$$

$$+ \quad \left[\langle\psi_0|G^\dagger(0z_1|0t_1)A\frac{\partial G(z_1^*0|t_10)}{\partial t_1}|\psi_0\rangle\right] \tag{8.1}$$

Replacing the evolution equation (7.46)of vacuum propagators,

$$\begin{aligned}
&\frac{d}{dt_1}\mathcal{M}_1\big[\langle\psi_0\mid G^\dagger(0z_1|0t_1)AG(z_1^*|t_10)\mid\psi_0\rangle\big] = \mathcal{M}_1\Bigg[\langle\psi_0\mid\Big\{G^\dagger(0z_1|0t_1)\big(iH_S+L^\dagger z_{1,t_1}\big)\\
&-\quad \int_0^{t_1}d\tau\alpha^*(t-\tau)\mathcal{M}_2\big[G^\dagger(0z_2|0\tau)L^\dagger G^\dagger(z_2^*z_1|\tau t_1)\big]L\Big\}AG(z_1^*0|t_10)\mid\psi_0\rangle\Bigg]\\
&+\quad \mathcal{M}_1\Bigg[\langle\psi_0\mid G^\dagger(0z_1|0t_1)A\Big\{\big(-iH_S+Lz^*_{1,t_1}\big)G(z_1^*0|t_10)\\
&-\quad L^\dagger\int_0^{t_1}d\tau\alpha(t_1-\tau)\mathcal{M}_2\big[G(z_1^*z_2|t_1\tau)LG(z_2^*|\tau0)\big]\Big\}\mid\psi_0\rangle\Bigg]
\end{aligned} \tag{8.2}$$

Let us now perform in the former equation the average in z_1 of the term

$$\mathcal{M}_1\left[z_{1,t_1}\langle\psi_0|G^\dagger(0z_1|0t_1)AG(z_1^*0|t_10)|\psi_0\rangle\right]. \tag{8.3}$$

It is shown in Appendix (I), that the functionals $\hat{\mathcal{W}}[t_{i+1},t_{i+1}]$ with initial condition such that

$$\frac{\partial\hat{\mathcal{W}}[t_{i+1},t_{i+1}]}{\partial z_i}=0 \tag{8.4}$$

have the following property,

$$\mathcal{M}_i\left[z_{i,t_i}\hat{\mathcal{W}}[t_i,t_{i+1}]\right]=\int_{t_{i+1}}^{t_i}d\tau\mathcal{M}_i\left[z_{i,t}z^*_{i,\tau}\right]\mathcal{M}_i\left[\left(\frac{\delta\hat{\mathcal{W}}[t_i,t_{i+1}]}{\delta z^*_{i,\tau}}\right)\right], \tag{8.5}$$

where it is assumed that z_{i,t_i} is a Gaussian noise of zero mean with the measure (2.5). This property can be used to evaluate (8.3), since $\hat{\mathcal{W}}[t_{i+1},t_{i+1}]=\hat{\mathcal{W}}[0,0]=\langle\psi_0|G^\dagger(0z_1|00)AG(z_1^*0|00)|\psi_0\rangle=\langle\psi_0|A|\psi_0\rangle$. Then the average of the first noise term is,

$$\begin{aligned}
&\mathcal{M}_1\left[z_{1,t_1}\langle\psi_0\mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_1^*0|t_10)\mid\psi_0\rangle\right]=\\
&\int_0^{t_1}d\tau\alpha(t_1-\tau)\mathcal{M}_1\Big[\langle\psi_0\mid G^\dagger(0z_1|0t_1)L^\dagger A\mathcal{M}_2\big[G(z_1^*z_2|t_1\tau)LG(z_2^*0|\tau0)\big]\mid\psi_0\rangle\Big].
\end{aligned} \tag{8.6}$$

Here we have used the expression

$$\begin{aligned}
\frac{\delta}{\delta z^*_{1,\tau}}G(z_1^*0|t_10) &= \langle z_1\mid\mathcal{U}_I(t_10)\mathcal{U}_I^{-1}(\tau,0)L\mathcal{U}_I(\tau,0)\mid0\rangle=\\
&= \mathcal{M}_2\left[G(z_1^*z_2|t_1\tau)LG(z_2^*0|\tau0)\right],
\end{aligned} \tag{8.7}$$

obtained in Appendix (K). In an analogous way, we get the following result for the average of the term with $z^*_{1,t}$,

$$\begin{aligned}
&\mathcal{M}_1\left[z^*_{1,t_1}\langle\psi_0\mid G^\dagger(0z_1|0t_1)ALG(z_1^*0|t_10)\mid\psi_0\rangle\right]=\\
&=\int_0^{t_1}d\tau\alpha^*(t_1-\tau)\mathcal{M}_1\left[\langle\psi_0\mid\mathcal{M}_2\big[G^\dagger(0z_2|0\tau)L^\dagger G^\dagger(z_2^*z_1|\tau t_1)\big]\right.\\
&\left.\times ALG(z_1^*0|t_10)\mid\psi_0\rangle\right].
\end{aligned} \tag{8.8}$$

Inserting equations (8.6) and (8.8) in (8.2), we obtain the following equation for one time correlations,

$$\begin{aligned}
& \mathcal{M}_1[\frac{d}{dt_1}\langle\psi_0 \mid G^\dagger(0z_1|0t_1)AG(z_1^*0|t_10) \mid \psi_0\rangle] = \\
= \;& \mathcal{M}_1\left[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)i[H_S,A]G(z_1^*0|t_10) \mid \psi_0\rangle\right] \\
+ \;& \int_0^{t_1} d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2}\left[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_1^*z_2|t_1\tau)LG(z_2^*0|\tau 0) \mid \psi_0\rangle\right] \\
- \;& \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\mathcal{M}_{1,2}\left[\langle\psi_0 \mid G^\dagger(0z_2|0\tau)L^\dagger G^\dagger(z_2^*z_1|\tau t_1)LAG(z_1^*0|t_10) \mid \psi_0\rangle\right] \\
+ \;& \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\mathcal{M}_{1,2}\left[\langle\psi_0 \mid G^\dagger(0z_2|0\tau)L^\dagger G^\dagger(z_2^*z_1|\tau t_1)LG(z_1^*0|t_10) \mid \psi_0\rangle\right] \\
- \;& \int_0^{t_1} d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2}\left[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)AL^\dagger G(z_1^*z_2|t_1\tau)LG(z_2^*0|\tau 0) \mid \psi_0\rangle\right]. \qquad (8.9)
\end{aligned}$$

Expressed in a simpler manner, the equation becomes,

$$\begin{aligned}
& \frac{d}{dt_1}\langle\Psi_0 \mid A(t_1) \mid \Psi_0\rangle = i\langle\Psi_0 \mid [H_S(t_1),A(t_1)] \mid \Psi_0\rangle \\
+ \;& \int_0^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid [L^\dagger(t_1),A(t_1)]L(\tau) \mid \Psi_0\rangle \\
+ \;& \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid L^\dagger(\tau)[A(t_1),L(t_1)] \mid \Psi_0\rangle. \qquad (8.10)
\end{aligned}$$

In the last expression it can be observed that the exact evolution of single mean values depends on two time correlations. Notice that this dependency is destroyed in the Markovian case, when the environmental correlation function $\alpha(t-\tau) = \Gamma\delta(t-\tau)$. Another possibility to break the dependency on higher correlations is to consider some approximation on the terms with two-time correlations. In Section (9.2.2), a perturbative approximation will be assumed, so that the equation (8.10) becomes a closed equation in terms of single mean values.

8.1.2 Evolution equation of two-time correlations

Let us now calculate the evolution equation for $C_{AB}(\mathbf{t}|\Psi_0) = \langle\Psi_0 \mid A(t_1)B(t_2) \mid \Psi_0\rangle$,

$$\begin{aligned}
\frac{dC_{AB}(\mathbf{t}|\Psi_0)}{dt_1} &= \mathcal{M}_{12}\left[\langle\psi_0|\frac{\partial G^\dagger(0z_1|0t_1)}{\partial t_1}AG(z_1^*z_2|t_1t_2)BG(z_2^*0|t_20)\rangle\right] \\
&+ \mathcal{M}_{12}\left[\langle\psi_0|G^\dagger(0z_1|0t_1)A\frac{\partial G(z_1^*z_2|t_1t_2)}{\partial t_1}BG(z_2^*|t_20)\rangle\right]. \qquad (8.11)
\end{aligned}$$

Inserting (7.46) and its complex conjugated, the following equation is obtained

$$\begin{aligned}
& \frac{d\langle\Psi_0 \mid A(t_1)B(t_2) \mid \Psi_0\rangle}{dt_1} = \mathcal{M}_{1,2}\Bigg[\langle\psi_0 \mid \Bigg\{G^\dagger(0z_1|0t_1)(iH_S + z_{1,t_1}L^\dagger) \\
- \;& \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\mathcal{M}_3\left[G^\dagger(0z_3|0\tau)L^\dagger G^\dagger(z_3^*z_1|\tau t_1)\right]L\Bigg\} \\
& \times AG(z_1^*z_2|t_1t_2)BG(z_2^*0|t_20) \mid \psi_0\rangle\Bigg]
\end{aligned}$$

$$\begin{aligned}
&+ \quad \mathcal{M}_{1,2}\Bigg[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)A\Bigg\{(-iH_S + z^*_{1,t_1}L - z_{2,t_1}L^\dagger)G(z_1^*z_2|t_1t_2) \\
&- \quad \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)\langle\psi_0 \mid G^\dagger(0z_1|0t_1)AL^\dagger\mathcal{M}_3\left[G(z_1^*z_3|t_1\tau)LG(z_3^*z_2|\tau t_2)\right]\Bigg\} \\
&\quad \times BG(z_2^*0|t_20) \mid \psi_0\rangle\Bigg]. \qquad (8.12)
\end{aligned}$$

Now, for functionals with initial condition such that $\partial\hat{\mathcal{W}}[t_{i+1},t_{i+1}]/\partial z_i = 0$, we have the property (8.5) for the average, and for functionals such that $\partial\mathcal{W}[t_{i+1},t_{i+1}]/\partial z_i = z_{i+1}$, we have

$$\mathcal{M}_i\left[z_{i,t_i}\mathcal{W}[t_i,t_{i+1}]\right] = z_{i+1,t_i}\mathcal{M}_i\left[\mathcal{W}[t_i,t_{i+1}]\right] + \int_{t_{i+1}}^{t_i} d\tau\mathcal{M}_i\left[z_{i,t}z^*_{i,\tau}\right]\mathcal{M}_i\left[\left(\frac{\delta\mathcal{W}[t_i,t_{i+1}]}{\delta z^*_{i,\tau}}\right)\right], \qquad (8.13)$$

as obtained in Appendix (I). Since the average of the noise term in z^*_{1,t_1} is performed with a functional of the first type we use the property (8.5),

$$\begin{aligned}
&\mathcal{M}_{1,2}\left[z^*_{1,t_1}\langle\psi_0 \mid G^\dagger(0z_1|0t_1)ALG(z_1^*z_2|t_1t_2)BG(z_2^*0|t_20) \mid \psi_0\rangle\right] \\
= \quad & \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\mathcal{M}_{1,2}\Bigg[\langle\psi_0 \mid \frac{\delta}{\delta z_{1,\tau}}G^\dagger(0z_1|0t_1) \\
& \times ALG(z_1^*z_2|t_1t)BG(z_2^*0|t_20) \mid \psi_0\rangle\Bigg] \\
= \quad & \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\mathcal{M}_{1,2,3}\Bigg[\langle\psi_0 \mid G^\dagger(0z_3|0\tau)L^\dagger G^\dagger(z_3^*z_1|\tau t_1) \\
& \times ALG(z_1^*z_2|t_1t_2)BG(z_2^*0|t_20) \mid \psi_0\rangle\Bigg]. \qquad (8.14)
\end{aligned}$$

Here, we have also considered the fact that the functional derivative can be in general expressed as,

$$\begin{aligned}
\frac{\delta G(z_i^*z_{i+1}|t_it_{i+1})}{\delta z^*_{i,\tau}} &= \langle z_i|\mathcal{U}_I(t_i,t_{i+1})L(\tau,t_{i+1})|z_{i+1}\rangle \\
= \quad & \mathcal{M}_l\left[G(z_i^*z_l|t_i\tau)LG(z_l^*z_{i+1}|\tau t_{i+1})\right]. \qquad (8.15)
\end{aligned}$$

The first equality appearing in the last expression is derived in Appendix (K), while the second equality, is obtained by expressing the evolution operators as reduced propagators with the insertion of a closure relation in a new variable z_l. The average of the term with z_{1,t_1} is performed by using the property (8.13) since the initial condition of the functional is $\exp\left(z_i^*z_{i+1}\right)$. Thus,

$$\begin{aligned}
&\mathcal{M}_{1,2}\left[z_{1,t_1}\langle\psi_0 \mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_1^*z_2|t_1t_2)BG(z_2^*|t_20) \mid \psi_0\rangle\right] \\
= \quad & \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3}\left[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)L^\dagger A\right. \\
& \left. G(z_1^*z_3|t_1\tau)LG(z_3^*z_2|\tau t_2)BG(z_2^*|t_20) \mid \psi_0\rangle\right] \\
+ \quad & \int_0^{t_2} d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3}\left[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)L^\dagger A\right. \\
& \left. G(z_1^*z_2|t_1t_2)BG(z_2^*z_3|t_2\tau)LG(z_3^*|\tau 0) \mid \psi_0\rangle\right]. \qquad (8.16)
\end{aligned}$$

In this expression we have also used (8.15). Finally, the average of the term with z_{2,t_1} is solved using again (8.5) together with (8.15),

$$\begin{aligned}
&\mathcal{M}_{1,2}\left[z_{2,t_1}\langle\psi_0 \mid G^\dagger(0z_1|0t_1)AL^\dagger G(z_l^* z_2|t_1t_2)BG(z_2^*|t_20) \mid \psi_0\rangle\right] \\
=\;& \int_0^{t_2} d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3}\Big[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)AL^\dagger \\
&\times G(z_1^* z_2|t_1t_2)BG(z_2^* z_3|t\tau)LG(z_3^*|\tau 0) \mid \psi_0\rangle\Big]. \qquad (8.17)
\end{aligned}$$

The replacement of (8.14), (8.16) and (8.17) in (8.12) gives the following evolution equation,

$$\begin{aligned}
&\frac{d\langle\Psi_0 \mid A(t_1)B(t_2) \mid \Psi_0\rangle}{dt_1} = i\langle\Psi_0 \mid [H_S(t_1),A(t_1)]B(t_2) \mid \Psi_0\rangle \\
+\;& \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid L^\dagger(\tau)[A(t_1),L(t_1)]B(t_2) \mid \Psi_0\rangle \\
+\;& \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid [L^\dagger(t_1),A(t_1)]L(\tau)B(t_2) \mid \Psi_0\rangle \\
+\;& \int_0^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid [L^\dagger(t_1),A(t_1)]B(t_2)L(\tau) \mid \Psi_0\rangle, \qquad (8.18)
\end{aligned}$$

that shows a dependency with three-time correlations.

8.1.3 Evolution equation of three time correlations

Let us now calculate the following evolution equation,

$$\begin{aligned}
&\frac{d\langle\Psi_0 \mid A(t_1)B(t_2)C(t_3) \mid \Psi_0\rangle}{dt_1} = \mathcal{M}_{1,2,3}\Bigg[\langle\psi_0 \mid \bigg\{G^\dagger(0z_1|0t_1)\big(iH_S + z_{1,t_1}L^\dagger\big) \\
-\;& \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\mathcal{M}_4\left[G^\dagger(0z_4|0\tau)L^\dagger G^\dagger(z_4^* z_1|\tau t_1)\right]L\bigg\} \\
&\times AG(z_1^* z_2|t_1t_2)BG(z_2^* z_3|t_2t_3)CG(z_3^* 0|t_30) \mid \psi_0\rangle\Bigg] \\
+\;& \mathcal{M}_{1,2,3}\Bigg[\langle\psi_0 \mid G^\dagger(0z_1|0t_1)A\bigg\{\big(-iH_S + z_{1,t_1}^* L - z_{2,t_1}L^\dagger\big)G(z_1^* z_2|t_1t_2) \\
-\;& \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)L^\dagger\mathcal{M}_4\left[G(z_1^* z_4|t_1\tau)LG(z_4^* z_2|\tau t_2)\right]\bigg\} \\
&BG(z_2^* z_3|t_2t_3)CG(z_3^* 0|t_30) \mid \psi_0\rangle.\Bigg] \qquad (8.19)
\end{aligned}$$

The average of the term with noise z_1^* is performed using the property (8.5) and the relation (8.15),

$$\begin{aligned}
&\mathcal{M}_{1,2,3}\left[z_{1,t_1}^*\langle\psi_0 \mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_l^* z_2|t_1t_2)BG(z_2^* z_3|t_2t_3)CG(z_3^* 0|t_30) \mid \psi_0\rangle\right] \\
=\;& \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\mathcal{M}_{1,2,3,4}\left[\langle\psi_0 \mid G^\dagger(0z_4|0\tau)L^\dagger G^\dagger(z_4^* z_1|\tau t_1)\right. \\
&\left.\times\; ALG(z_1^* z_2|t_1t_2)BG(z_2^* z_3|t_2t_3))CG(z_3^* 0|t_30) \mid \psi_0\rangle\right] \qquad (8.20)
\end{aligned}$$

Using the Novikov property (8.13) and the relation (8.15), we get the following result for the average of the term z_{1,t_1},

$$\begin{aligned}
&\mathcal{M}_{1,2,3}\left[z_{1,t_1}\langle\psi_0\mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_l^*z_2|t_1t_2)BG(z_2^*z_3|t_2t_3)CG(z_3^*0|t_30)\mid\psi_0\rangle\right]\\
=\;&\int_{t_2}^{t_1}d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3,4}\left[\langle\psi_0\mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_1^*z_4|t_1\tau)LG(z_4^*z_2|\tau t_2)\right.\\
&\times BG(z_2^*z_3|t_2t_3)CG(z_3^*0|t_30)\mid\psi_0\rangle]\\
+\;&\int_{t_3}^{t_2}d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3,4}\left[\langle\psi_0\mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_1^*z_2|t_1t_2)\right.\\
&BG(z_2^*z_4|t\tau)LG(z_4^*z_3|\tau t_3)CG(z_3^*0|t_30)\mid\psi_0\rangle]\\
+\;&\int_{0}^{t_3}d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3,4}\left[\langle\psi_0\mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_1^*z_2|t_1t_2)\right.\\
&\times BG(z_2^*z_3|t_2t_3)CG(z_3^*z_4|t_3\tau)LG(z_4^*0|\tau 0)\mid\psi_0\rangle]\,. \qquad (8.21)
\end{aligned}$$

Finally, in an analogous way, using the same properties we can calculate the following average,

$$\begin{aligned}
&\mathcal{M}_{1,2,3}\left[z_{2,t_1}\langle\psi_0\mid G^\dagger(0z_1|0t_1)AL^\dagger G(z_l^*z_2|t_1t_2)BG(z_2^*z_3|t_2t_3)CG(z_3^*0|t_30)\mid\psi_0\rangle\right]\\
+\;&\int_{t_3}^{t_2}d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3,4}\left[\langle\psi_0\mid G^\dagger(0z_1|0t_1)L^\dagger AG(z_1^*z_2|t_1t_2)\right.\\
&\times BG(z_2^*z_4|t\tau)LG(z_4^*z_3|\tau t_3)CG(z_3^*0|t_30)\mid\psi_0\rangle]\\
+\;&\int_{0}^{t_3}d\tau\alpha(t_1-\tau)\mathcal{M}_{1,2,3,4}\left[\langle\psi_0\mid G^\dagger(0z_1|0t_1)AL^\dagger G(z_1^*z_2|t_1t_2)\right.\\
&\times BG(z_2^*z_3|t_2t_3)CG(z_3^*z_4|t_3\tau)LG(z_4^*0|\tau 0)\mid\psi_0\rangle]\,. \qquad (8.22)
\end{aligned}$$

The replacement of (8.20), (8.21) and (8.22) in (8.19) gives rise to the following equation for three time correlations,

$$\begin{aligned}
&\frac{d\langle\Psi_0\mid A(t_1)B(t_2)C(t_3)\mid\Psi_0\rangle}{dt_1}=i\langle\{[H_S,A]\}(t_1)B(t_2)C(t_3)\rangle\\
+\;&\int_0^{t_1}d\tau\alpha^*(t_1-\tau)\langle\Psi_0\mid L^\dagger(\tau)[A(t_1),L(t_1)]B(t)C(t_3)\mid\Psi_0\rangle\\
+\;&\int_{t_2}^{t_1}d\tau\alpha(t_1-\tau)\langle\Psi_0\mid[L^\dagger(t_1),A(t_1)]L(\tau)B(t_2)C(t_3)\mid\Psi_0\rangle\\
+\;&\int_{t_3}^{t_2}d\tau\alpha(t_1-\tau)\langle\Psi_0\mid[L^\dagger(t_1),A(t_1)]B(t_2)L(\tau)C(t_3)\mid\Psi_0\rangle\\
+\;&\int_{0}^{t_3}d\tau\alpha(t_1-\tau)\langle\Psi_0\mid[L^\dagger(t_1),A(t_1)]B(t_2)C(t_3)L(\tau)\mid\Psi_0\rangle. \qquad (8.23)
\end{aligned}$$

This equation shows how the evolution of non-Markovian three-time correlations depends in principle on four-time correlations.

8.2 METHOD II: MTCF IN THE HEISENBERG FORMALISM.

In this section we show how the equations obtained in the former section can also be derived within the Heisenberg formalism. The idea is to express $dA_1(t_1)\cdots A_N(t_N)/dt_1$ in such a way that the environmental operators $a_\lambda(0)$ are placed on the right hand side of the terms, while the $a^\dagger_\lambda(0)$ appear in the left hand side. Thus, when we compute the MTCF as the quantum mean value of $A_1(t_1)\cdots A_N(t_N)$, i.e. as $C_{\mathbf{A}}(\mathbf{t}|\Psi_0) = \langle\psi_0|\langle 0|A_1(t_1)\cdots A_N(t_N)|0\rangle|\psi_0\rangle$, where we have considered $\rho_{tot}(0) = |\psi_0\rangle\langle\psi_0|\otimes|0\rangle\langle 0|$, those terms are zero, and only system operators appear in the equations. Let us consider the Heisenberg evolution equation for a system observable $A(t) = \mathcal{U}^{-1}(t,0)A\mathcal{U}(t,0)$, where $\mathcal{U}(t,0)$ is the evolution operator with the total Hamiltonian (7.40),

$$\begin{aligned} \frac{dA(t_1)}{dt_1} &= i\mathcal{U}^{-1}(t_1,0)[H_{tot},A]\mathcal{U}(t_1,0) = -i[H_S(t_1),A(t_1)] \\ &+ \quad i\sum_\lambda g_\lambda\left(a^\dagger_\lambda(t_1,0)[L(t_1),A(t_1)] + [L^\dagger(t_1),A(t_1)]a_\lambda(t_1,0)\right), \end{aligned} \tag{8.24}$$

We can replace in (8.24) the formal solution of the evolution equation of the environmental operators, $da_\lambda(t_1,0)/dt_1 = i[H_{tot}(t_1),a_\lambda(t_1,0)] = -i\omega_\lambda a_\lambda(t_1,0) - ig_\lambda L(t_1)$,

$$a_\lambda(t_1,0) = e^{-i\omega_\lambda t_1}a(0,0) - ig_\lambda\int_0^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau). \tag{8.25}$$

The single evolution equation (8.24) becomes as follows,

$$\begin{aligned} \frac{dA(t_1)}{dt_1} &= i[H_S(t_1),A(t_1)] - \nu^\dagger(t_1)[L(t_1),A(t_1)] \\ &+ \quad \int_0^{t_1} d\tau\alpha^*(t_1-\tau)L^\dagger(\tau)[A(t_1),L(t_1)] + [L^\dagger(t_1),A(t_1)]\nu(t_1) \\ &+ \quad \int_0^{t_1} d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]L(\tau), \end{aligned} \tag{8.26}$$

where we have used the definition (7.48) of the environment correlation function. In the last expression, we have also defined, like in Chapter (2) the bath operators

$$\begin{aligned} \nu^\dagger(t_1) &= -i\sum_\lambda g_\lambda a^\dagger_\lambda(0,0)e^{i\omega_\lambda t_1} \\ \nu(t_1) &= i\sum_\lambda g_\lambda a_\lambda(0,0)e^{-i\omega_\lambda t_1} \end{aligned} \tag{8.27}$$

It is easy to see from (8.26) that the evolution equation of the quantum mean value of A, provided that the total initial state is $|\Psi_0\rangle = |\psi_0\rangle\ |0\rangle$, is equal to the equation (8.10) derived in last section through the system propagators formalism. Let us now calculate the following evolution equation,

$$\begin{aligned} \frac{dA(t_1)B(t_2)}{dt} &= i\mathcal{U}^{-1}(t_1)[H_{tot},A]\mathcal{U}(t_1)B(t) = i[H_S(t_1),A(t_1)]B(t_2) \\ &+ \quad i\sum_\lambda g_\lambda\left(a^\dagger_\lambda(t_1,0)[L(t_1),A(t_1)]B(t_2) + [L^\dagger(t_1),A(t_1)]a_\lambda(t_1,0)B(t_2)\right). \end{aligned} \tag{8.28}$$

The idea is again to eliminate the dependency on the environmental operators once the average over the total system state is performed. First, we again replace the analytical solution of the creation operator $a^\dagger_\lambda(t_1,0)$, so that the term $a^\dagger_\lambda(0,0)$ appears in the left hand side of the expression and can be eliminated when applying the vacuum initial state. Second, we move the annihilation operator to the right hand side by doing the following,

$$\begin{aligned} a_\lambda(t_1,0)B(t_2) &= \mathcal{U}^{-1}(t_2)a_\lambda(t_1,t_2)B\mathcal{U}(t_2) \\ &= \mathcal{U}^{-1}(t_2)e^{-i\omega_\lambda(t_1-t_2)}a_\lambda(0,0)B\mathcal{U}(t_2) - ig_\lambda\int_{t_2}^{t_1}d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2) \\ &= B(t_2)a_\lambda(t_2,0) - ig_\lambda\int_{t_2}^{t_1}d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2) \end{aligned} \tag{8.29}$$

where we have used

$$a_\lambda(t_1,t_2) = e^{-i\omega_\lambda(t_1-t_2)}a_\lambda(t_2,t_2) - ig_\lambda\int_{t_2}^{t_1}d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau,t_2), \tag{8.30}$$

with $a_\lambda(t_2,t_2) = a_\lambda(0,0) \equiv a_\lambda$, and $[B, a_\lambda(0,0)] = 0$. We now insert in the former expression the solution of $a_\lambda(t_2,0)$, which is of the form (8.25), and obtain

$$\begin{aligned} a_\lambda(t_1,0)B(t_2) &= e^{-i\omega_\lambda t_1}B(t_2)a_\lambda(0,0) - ig_\lambda\int_0^{t_2}d\tau e^{-i\omega_\lambda(t_1-\tau)}B(t_2)L(\tau) \\ &- ig_\lambda\int_{t_2}^{t_1}d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2). \end{aligned} \tag{8.31}$$

Replacing (8.31) in (8.28), and considering the solution of $a^\dagger_\lambda(t_1,0)$, we obtain the following

$$\begin{aligned} \frac{dA(t_1)B(t_2)}{dt_1} &= i[H_S(t_1),A(t_1)]B(t_2) - \nu^\dagger(t_1)[L(t_1),A(t_1)]B(t_2) \\ &- \int_0^{t_1}d\tau\alpha^*(t_1-\tau)L^\dagger(\tau)[L(t_1),A(t_1)]B(t_2) + [L^\dagger(t_1),A(t_1)]B(t_2)\nu(t_1) \\ &+ \int_{t_2}^{t_1}d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]L(\tau)B(t_2) + \int_0^{t_2}d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]B(t_2)L(\tau). \end{aligned} \tag{8.32}$$

The evolution of the quantum mean value $\langle A(t_1)B(t_2)\rangle$ is again obtained by applying the total initial state on both sides of the former expression. When such initial state is $\mid\psi_0\rangle\mid 0\rangle$, we again obtain the same result as with the method of system propagators, i.e. equation (8.18). For triple correlations, we start from

$$\begin{aligned} \frac{dA(t_1)B(t_2)C(t_3)}{dt_1} &= i\mathcal{U}^{-1}(t_1)[H_{tot},A]\mathcal{U}(t_1)B(t_2)C(t_3) \\ &= i[H_S(t_1),A(t_1)]B(t_2)C(t_3) + i\sum_\lambda g_\lambda\Big(a^\dagger_\lambda(t_1,0)[L(t_1),A(t_1)]B(t_2)C(t_3) \\ &+ [L^\dagger(t_1),A(t_1)]a_\lambda(t_1,0)B(t_2)C(t_3)\Big). \end{aligned} \tag{8.33}$$

While the term with $a^\dagger_\lambda(t_1,0)$ can be treated by simply replacing the solution of its Heisenberg equation, the term with the combination $a_\lambda(t_1,0)B(t)C(t_3)$ needs further simplification,

$$a_\lambda(t_1,0)B(t_2)C(t_3) =$$

$$
\begin{aligned}
&= \mathcal{U}^{-1}(t_2)e^{-i\omega_\lambda(t_1-t_2)}a_\lambda(0,0)B\mathcal{U}(t_2)C(t_3) - ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2)C(t_3)\\
&= e^{-i\omega_\lambda(t_1-t_2)}B(t_2)\mathcal{U}^{-1}(t_3)a(t_2,t_3)C\mathcal{U}(t_3) - ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2)C(t_3)\\
&= B(t_2)C(t_3)a_\lambda(0,0)e^{-i\omega_\lambda t_1} - ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2)C(t_3)\\
&- ig_\lambda\int_{t_3}^{t_2} d\tau e^{-i\omega_\lambda(t_1-\tau)}B(t_2)L(\tau)C(t_3)\\
&- ig_\lambda\int_{0}^{t_3} d\tau e^{-i\omega_\lambda(t_1-\tau)}B(t_2)C(t_3)L(\tau). \qquad (8.34)
\end{aligned}
$$

Inserting the last expression in (8.33), and the expression for $a_\lambda^\dagger(t_1,0)$, we get the following equation,

$$
\begin{aligned}
&\frac{dA(t_1)B(t_2)C(t_3)}{dt_1} = i[H_S(t_1),A(t_1)]B(t_2)C(t_3)\\
&- \nu^\dagger(t_1)[L(t_1),A(t_1)]B(t_2)C(t_3) + [L^\dagger(t_1),A(t_1)]B(t_2)C(t_3)\nu(t_1)\\
&+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)L^\dagger(\tau)[A(t_1),L(t_1)]B(t_2)C(t_3)\\
&+ \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]L(\tau)B(t_2)C(t_3)\\
&+ \int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]B(t_2)L(\tau)C(t_3)\\
&+ \int_{0}^{t_3} d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]B(t_2)C(t_3)L(\tau) \qquad (8.35)
\end{aligned}
$$

Since the annihilation operators $a_\lambda(0,0)$ are on the right, and the creation operators $a_\lambda^\dagger(0,0)$ are on the left, this expression is identical to equation (8.23), once the initial state for the total wave vector, $|\Psi_0\rangle = |\psi_0\rangle|0\rangle$, is applied.

8.3 GENERALIZATION TO A N-TIME CORRELATION FUNCTION

The evolution equations presented in Sections (8.1) and (8.2) with the reduced propagator and the Heisenberg equation method respectively, can be generalized to N-time correlations. The reason is that the different terms of the equation, as well as their corresponding integration limits are ordered in a sequence. To see this more clearly, let us consider the following string of operators $\{L(\tau)A_2(t_2)\cdots A_N(t_N)\} = L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})$, where $\tilde{\mathbf{t}}^{(\mathbf{2})} = \{t_2\cdots t_N\}$, and we have defined

$$
\tilde{\mathbf{A}}^{(\mathbf{n})}(\tilde{\mathbf{t}}^{(\mathbf{n})}) = A_n(t_n)\cdots A_N(t_N), \qquad (8.36)
$$

with $\tilde{\mathbf{t}}^{(\mathbf{n})} = \{t_n\cdots t_N\}$. We define a displacement superoperator $\mathcal{P}_R$ that translate the operator $L(\tau)$ *to the right* one place inside the string $\tilde{\mathbf{A}}(\tilde{\mathbf{t}})$. In such terms, we have

$$
\frac{d\mathbf{A}(\mathbf{t})}{dt_1} = i[H_S(t_1),A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})
$$

$$
\begin{aligned}
&- \nu^\dagger(t_1)[L(t_1),A(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) + [L^\dagger(t_1),A(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})\nu(t_1) \\
&+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)L^\dagger(\tau)[A_1(t_1),L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \\
&+ \sum_{i=0}^{N-1}\int_{t_{i+2}}^{t_{i+1}} d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A_1(t_1)]\mathcal{P}_R^i L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})
\end{aligned} \tag{8.37}
$$

and the evolution equation for the N-time correlation function for $\rho_{tot}(0)=|\Psi_0\rangle\langle\Psi_0|=|\psi_0\rangle\langle\psi_0|\otimes|0\rangle\langle 0|$ reads as follows,

$$
\begin{aligned}
&\frac{dC_{\mathbf{A}}(\mathbf{t}|\Psi_0)}{dt_1} = i\langle\Psi_0 \mid [H_S(t_1),A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\
&+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid L^\dagger(\tau)[A_1(t_1),L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\
&+ \sum_{i=0}^{N-1}\int_{t_{i+2}}^{t_{i+1}} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid [L^\dagger(t_1),A_1(t_1)]\mathcal{P}_R^i L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle
\end{aligned} \tag{8.38}
$$

Notice that here, the displacement operator is defined in such a way that

$$
\begin{aligned}
&\mathcal{P}_R^0 L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) = L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \\
&\mathcal{P}_R^1 L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) = A_2(t_2)L(\tau)\tilde{\mathbf{A}}^{(\mathbf{3})}(\tilde{\mathbf{t}}^{(\mathbf{3})}) \\
&\mathcal{P}_R^2 L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) = A_2(t_2)A_3(t_3)L(\tau)\tilde{\mathbf{A}}^{(\mathbf{4})}(\tilde{\mathbf{t}}^{(\mathbf{4})}) \\
&\ldots \\
&\mathcal{P}_R^{N-1} L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) = \tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})L(\tau).
\end{aligned} \tag{8.39}
$$

Replacing $N=0$, $N=1$ and $N=2$ in (8.38), the one-time evolution equation (8.10), the two-time evolution equation (8.18), and the three-time evolution equation (8.23) is obtained respectively [1].

---

[1] It should be reminded that the initial time, $t_0 = t_{N+1} = 0$.

9

Non-Markovian MTCF up to second order in perturbation parameter.

In this chapter we discuss three different methods to derive MTCF up to second order in the coupling constant.

The first, treated in Section (9.1), is essentially *numeric*, and consists in making an ensemble average of different stochastic trajectories. These trajectories are obtained by using the second order perturbative equation for the reduced propagator (7.50), in which $O(z_{i+1}z_i^*, t, \tau) = V_{t-\tau}L$.

The other two methods consist in deriving a set of coupled differential equations for MTCF: In Section (9.2.1) such set is obtained by using a weak coupling expansion of the reduced propagator, and then performing *analytically* the average over the environmental variables z_{i+1} and z_i. In Section (9.2.2), a third method is presented which consists in applying the second order perturbative hypothesis to the hierarchy of evolution equations derived in the last chapter. As noted before, in order to use the hierarchy for computational purposes and not just as a formal derivation, the dependency on higher order correlations should be broken. This is done in this chapter by applying a second perturbative hypothesis directly on the N-time correlation we want to compute, so that its dependency on the $N+1$-time correlations vanishes.

9.1 COMPUTING SECOND ORDER MTCFS WITH STOCHASTIC SAMPLING

The solutions of the equations of motion for the reduced propagators, once they are replaced in (7.44), are the starting point to compute correlation functions. Once the noises, i.e. the set of coherent states appearing (7.44), $\{z_i = z_{i,1} \cdots z_{i,\lambda} \cdots\}$ for $i = 0, \cdots, N+1$, has been chosen, the element

$$\langle\psi_0|G^\dagger(z'^* z_1|0t_1)\prod_{i=1}^{N} A_i G(z_i^* z_{i+1}|t_i t_{i+1})|\psi_0\rangle, \tag{9.1}$$

can be integrated. If for instance we want to compute numerically two-time correlations, it is necessary to make an average with the functions $\langle\psi_0|G^\dagger(z_1|0t_1)AG(z_1^* z_2|t_1t_2)BG(z_2^*|t_2 0)|\psi_0\rangle$ for different noise histories. To construct each function, the following steps have to be taken:

- Propagate $G(z_2^*|t_2 0)|\psi_0\rangle$ from 0 to t_2, choosing randomly the set of $z_{2,\lambda}$ appearing in the function z_{2,t_2}. This choice is made according to a Gaussian distribution $d\mu(z) = \prod_{\lambda=1}^{\nu}(d^2 z_\lambda \exp(-|z_\lambda|^2))/\pi$, where ν is the number of environmental modes we consider. In the same way, chose the set of $\{z_{1,\lambda}\}$, and evolve the function $|\ \psi_{t_2}(z_1^* 0)\rangle = G(z_1^*|t_2 0)|\psi_0\rangle$;
- Apply the matrix B to the wave function evolving with z_2, so that we obtain $|\ \phi_{t_2}(z_2^*)\rangle = BG(z_2^* 0|t_2 0)|\psi_0\rangle$.
- Propagate from t_2 to t_1 the functions $|\ \psi_{t_2}(z_1^*)\rangle$ and $|\ \phi_{t_2}(z_2^*)\rangle$. The first one is evolved just continuing with the evolution given by the vacuum propagator, while the evolution of the second one has to be performed by applying the propagator $G(z_1^* z_2|t_1 t_2)$, that gives a wave function $|\ \phi_{t_1,t_2}(z_2^*, z_1^*, z_2)\rangle = G(z_1^* z_2|t_1 t_2)\ |\ \phi_{t_2}(z_2^*)\rangle$. It is important to stress that the noises z_{1,t_1} and z_{2,t_1} appearing in the evolution of the propagator are calculated respectively with the sets $\{z_{1,\lambda}\}$ and $\{z_{2,\lambda}\}$ already chosen. Another important point is to take into account that the propagator has as initial condition $G(z_1^* z_2|t_2 t_2) = \exp(z_1^* z_2)$, with $z_1^* z_2 = \sum_\lambda z_{1,\lambda}^* z_{2,\lambda}$.
- Reconstruct $\langle\psi_0|G^\dagger(z_1|0t_1)AG(z_1^* z_2|t_1 t_2)BG(z_2^*|t_2 0)|\psi_0\rangle$ with $\langle\psi_{t_1}(z_1)\ |\ A\ |\ \phi_{t_1,t_2}(z_2^*, z_1^*, z_2)\rangle$.

This steps are repeated as many times as needed to obtain a good sampling of (7.44). The figure (9.1) is represents an scheme of these steps.

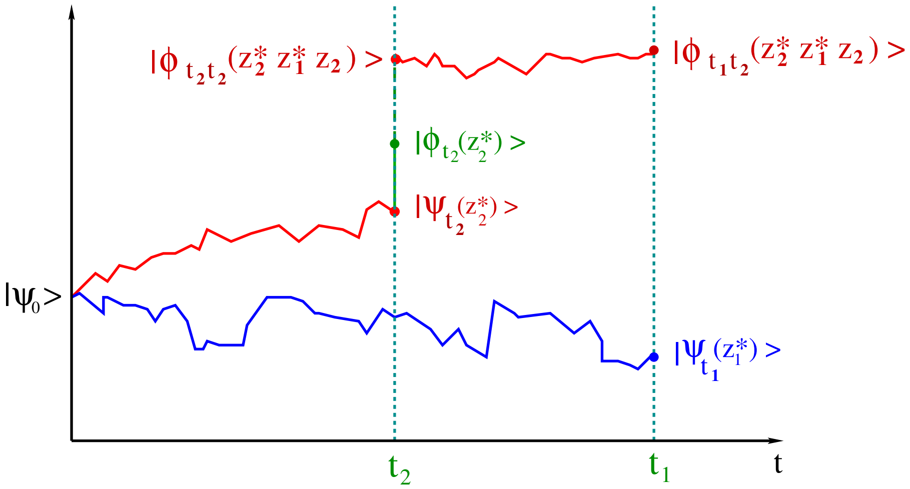

Fig. 9.1 Schematic evolution of the two vectors, $|\psi_{t_1}(z_1)\rangle$ (in blue), and $|\ \phi_{t_1,t_2}(z_2^*, z_1^*, z_2)\rangle$ (in red), needed to obtain one single stochastic value of the element $\langle\psi_{t_1}(z_1)\ |\ A\ |\ \phi_{t_1,t_2}(z_2^*, z_1^*, z_2)\rangle$. A sum of different elements, obtained with an ensemble of noise values of $z_{1,t}$ and $z_{2,t}$ gives rise to the desired two time correlation function $\langle\Psi_0\ |\ A(t_1)B(t_2)\ |\ \Psi_0\rangle$.

9.2 COMPUTING MTCF WITH A SET OF COUPLED DIFFERENTIAL EQUATIONS

Once we have the multiple time correlation functions, we may compute them directly from the stochastic method. Nonetheless, this may turn to be an expensive strategy from the numerical point of view, which is particularly true when the number of environmental degrees of freedom needed to correctly describe its correlation function is large. Therefore, it may be convenient to have a set of differential equations from which the MTCF may be obtained, and where the stochastic average has been performed analytically. In this section, we calculate such a set of coupled differential equations which evolve, up to second order in a convenient perturbation parameter g, the non-Markovian two-time correlations. We also show how to calculate such set of coupled equations from the hierarchy of equations derived in the Chapter (8), and derive the general equation for N-time correlation functions up to second order. Finally, it will be shown that only under several conditions do these equations reduce to those of the Quantum Regression Theorem. This chapter ends with the application of the two-time correlation functions to a solvable example, a dissipative system with exponential correlation function and a spin-boson model. In those examples the equivalence of using a stochastic sampling and using the set of coupled differential equations is shown. The choice of the stochastic method or the system of equations for computing the MTCF has to be made according to the particular problem. When evolving quantum mean values we saw that for a system with a large number of degrees of freedom, $\mathcal{F}$, the stochastic method is generally more convenient, since in the dimension of the density matrix grows with $\mathcal{F}^2$. The same happens in MTCF. When a N-time correlation function has to be computed, the quantity that should be taken into account is the number $\mathcal{Y}$ of matrices that form a basis for the QOS. The correlation of other system observables can be computed by combining correlations of this basic set of observables. As an example,for a two level system the basis is $\{\sigma_x, \sigma_y, \sigma_z\}$, so that $\mathcal{Y} = 3$. In that case, stochastic method permit us to compute only the particular correlation function that is needed, and not the whole set of $\mathcal{Y}^N$ correlations that appears interrelated in the set of differential equations.

9.2.1 Computing MTCF with the weak coupling expansion

The method we will follow consists in deriving the stochastic two-time correlation with respect to t_1,

$$\begin{aligned}
&\frac{d}{dt_1}\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) A G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle = \\
&\langle\psi_0 \mid \left(\frac{d}{dt_1} G^\dagger(z_1 0|t_1 0)\right) A G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle \\
+ \quad &\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) A \left(\frac{d}{dt_1} G(z_1^* z_2|t_1 t_2)\right) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle \qquad (9.2)
\end{aligned}$$

and then performing analytically the average over the variables z_1 and z_2. The first derivative appearing in (9.2) corresponds to the hermitian conjugate of the usual equation for the vacuum propagator, which reads as follows,

$$\frac{d}{dt_1} G(z_1^* 0|t_1 0) = \left\{-iH_S + L z_{1,t_1}^* - L^\dagger \int_0^{t_1} d\tau \alpha(t_1 - \tau) V_{\tau - t_1} L\right\} G(z_1^* 0|t_1 0) + \mathcal{O}(g^3). \qquad (9.3)$$

The second term is given by the equation,

$$\frac{d}{dt_1} G(z_1^* z_2|t_1 t_2) = \left\{-iH_S + L z_{1,t_1}^* - L^\dagger z_{2,t_1} - L^\dagger \int_{t_2}^{t_1} d\tau \alpha(t_1 - \tau) V_{\tau - t_1} L\right\} G(z_1^* z_2|t_1 t_2) + \mathcal{O}(g^3), (9.4)$$

presented in previous sections. Inserting the last expressions in (9.2), we find that

$$\begin{aligned}
&\frac{d}{dt_1}\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) A G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle = \\
+ \quad & i\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) [H_S, A] G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle \\
- \quad & \int_0^{t_1} d\tau \alpha^*(t_1 - \tau) \langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) V_{\tau - t_1} L^\dagger L A G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle
\end{aligned}$$

$$\begin{aligned}
&- \int_{t_2}^{t_1} d\tau \alpha(t_1-\tau)\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) A L^\dagger V_{\tau-t_1} L G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle \\
&+ z_{1,t_1}\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) L^\dagger A G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle \\
&+ z_{1,t_1}^*\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) A L G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle \\
&- z_{2,t_1}^*\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) A L^\dagger G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle. \qquad (9.5)
\end{aligned}$$

In order to make the averages, we will handle second order perturbative expansions of these evolution operators, which are

$$\begin{aligned}
G(z_1^* 0|t_1 0) = \Big\{ 1 &+ \int_0^{t_1} d\tau z_{1,\tau}^* V_{\tau-t_1} L + \int_0^{t_1} d\tau \int_0^{\tau} d\tau' z_{1,\tau}^* z_{1,\tau'}^* V_{\tau-t_1} L V_{\tau'-t_1} L \\
&- \int_0^{t_1} d\tau \int_0^{\tau} d\tau' \alpha(\tau-\tau') V_{\tau-t_1} L^\dagger V_{\tau'-t_1} L \Big\} G^{(0)}(z_1^* 0|t_1 0) + \mathcal{O}(g^3), \qquad (9.6)
\end{aligned}$$

for (9.3), where $G^{(0)}(z_1^* 0|t_1 0) = \exp(-iH_S t_1)$ represent the zero order in the perturbative expansion, and

$$\begin{aligned}
G(z_1^*, z_2|t_1 t_2) &= \Big\{ 1 + \int_{t_2}^{t_1} d\tau z_{1,\tau}^* V_{\tau-t_1} L - \int_{t_2}^{t_1} d\tau z_{2,\tau} V_{\tau-t_1} L^\dagger \\
&- \int_{t_2}^{t_1} d\tau \int_{t}^{\tau} d\tau' \alpha(\tau-\tau') V_{\tau-t_1} L^\dagger V_{\tau'-t_1} L + \int_{t}^{t_1} d\tau \int_{t}^{\tau} d\tau' z_{1,\tau}^* z_{1,\tau'}^* V_{\tau-t_1} L V_{\tau'-t_1} L \\
&- \int_{t}^{t_1} d\tau \int_{t_2}^{\tau} d\tau' z_{1,\tau}^* z_{2,\tau'} V_{\tau-t_1} L V_{\tau'-t_1} L^\dagger - \int_{t_2}^{t_1} d\tau \int_{t_2}^{\tau} d\tau' z_{2,\tau} z_{1,\tau'}^* V_{\tau-t_1} L^\dagger V_{\tau'-t_1} L \\
&- \int_{t_2}^{t_1} d\tau \int_{t_2}^{\tau} d\tau' z_{2,\tau} z_{2,\tau'} V_{\tau-t_1} L^\dagger V_{\tau'-t_1} L^\dagger \Big\} G^{(0)}(z_1^*, z_2|t_1 t_2) + \mathcal{O}(g^3), \qquad (9.7)
\end{aligned}$$

for (9.4), where now the zero order is $G^{(0)}(z_1^* z_2|t_1 t_2) = \exp(-iH_S(t_1-t_2))\exp(z_1^* z_2)$. The average of term in z_{1,t_1} is such that

$$\begin{aligned}
&\int d\mu(z_1) \int d\mu(z_2) z_{1,t_1}\langle\psi_0 \mid G^\dagger(z_1 0|t_1 0) L^\dagger A G(z_1^* z_2|t_1 t_2) B G(z_2^* 0|t_2 0) \mid \psi_0\rangle = \\
= &\int d\mu(z_1) \int d\mu(z_2) z_{1,t_1}\langle\psi_0 \mid G^{\dagger,(0)}(0 z_1|0 t_1) \Big\{ 1 + \int_0^{t_1} d\tau z_{1,\tau} V_{\tau-t_1} L^\dagger \Big\} L^\dagger A \\
&\times \Big\{ 1 + \int_{t_2}^{t_1} d\tau z_{1,\tau}^* V_{\tau-t_1} L - \int_{t_2}^{t_1} d\tau z_{2,\tau} V_{\tau-t_1} L^\dagger \Big\} B \Big\{ 1 + \int_0^{t_1} d\tau z_{1,\tau}^* V_{\tau-t_1} L \Big\} \mid \psi_0\rangle \\
+ &\ \mathcal{O}(g^3), \qquad (9.8)
\end{aligned}$$

where we have inserted the perturbative expansions of the propagators, (9.6) and (9.7) up to first order in g, since the term is already of first order. The Gaussian integrals, are in fact multi-dimensional integrals over the coordinates of each harmonic oscillator of the environment. Four types of them have to be computed,

$$\begin{aligned}
&\int d\mu(z_{2,\lambda}) \int d\mu(z_{1,\lambda}) z_{1,\lambda} z_{1,\lambda} e^{z_{1,\lambda}^* z_{2,\lambda}} = 0 \\
&\int d\mu(z_{2,\lambda}) \int d\mu(z_{1,\lambda}) z_{1,\lambda} z_{1,\lambda}^* e^{z_{1,\lambda}^* z_{2,\lambda}} = 1
\end{aligned}$$

$$\begin{aligned}
\int d\mu(z_{2,\lambda}) \int d\mu(z_{1,\lambda}) z_{1,\lambda} z^*_{2,\lambda} e^{z^*_{1,\lambda} z_{2,\lambda}} &= \int d\mu(z_{1,\lambda}) z_{1,\lambda} z^*_{1,\lambda} = 1 \\
\int d\mu(z_{2,\lambda}) \int d\mu(z_{1,\lambda}) z_{1,\lambda} z_{2,\lambda} e^{z^*_{1,\lambda} z_{2,\lambda}} &= \int d\mu(z_{1,\lambda}) z_{1,\lambda} z_{1,\lambda} = 0
\end{aligned} \tag{9.9}$$

what give rise to the following result,

$$\begin{aligned}
& \int d\mu(z_1) \int d\mu(z_2) z_{1,t_1} \langle \psi_0 \mid G^\dagger(0 z_1 | 0 t_1) L^\dagger A G(z_1^* z_2 | t_1 t_2) B G(z_2^* 0 | t_2 0) \mid \psi_0 \rangle = \\
& \int_{t_2}^{t_1} d\tau \alpha(t_1 - \tau) \langle \psi_0 | e^{iH_S t_1} L^\dagger A V_{\tau - t_1} L e^{-iH_S(t_1 - t_2)} B e^{-iH_S t_2} | \psi_0 \rangle \\
+ \; & \int_0^{t_2} d\tau \alpha(t_1 - \tau) \langle \psi_0 | e^{iH_S t_1} | L^\dagger A e^{-iH_S(t_1 - t_2)} B V_{\tau - t_1} L e^{-iH_S t_2} | \psi_0 \rangle .
\end{aligned} \tag{9.10}$$

Since the quantities $e^{iH_S t_1}$, $e^{-iH_S(t_1-t_2)}$ and $e^{-iH_S t_2}$ represent the Gaussian averages over z_1 and z_2 of the first order term of the perturbative expansion of $G^\dagger(0z_1|0t_1)$, $G(z_1^* z_2|t_1 t_2)$ and $G(z_2^* 0|t_2 0)$ respectively, we conclude that the last terms can be written as

$$\begin{aligned}
& \int d\mu(z_1) \int d\mu(z_2) z_{1,t_1} \langle \psi_0 \mid G^\dagger(0 z_1 | 0 t_1) L^\dagger A G(z_1^* z_2 | t_1 t_2) B G(z_2^* 0 | t_2 0) \mid \psi_0 \rangle = \\
& \int_{t_2}^{t_1} d\tau \alpha(t_1 - \tau) \langle \Psi_0 | \left\{ L^\dagger A V_{\tau - t_1} L \right\} (t_1) B(t_2) | \Psi_0 \rangle \\
+ \; & \int_0^{t_2} d\tau \alpha(t_1 - \tau) \langle \Psi_0 \left\{ L^\dagger A \right\} (t_1) \left\{ B V_{\tau - t_1} L \right\} (t_2) | \Psi_0 \rangle .
\end{aligned} \tag{9.11}$$

The brackets involving a group of operators denote that the evolution affects all of them, $\{ABC\}(t_1) = \mathcal{U}_I^{-1}(t_1, 0) ABC \mathcal{U}_I(t_1, 0) = A(t_1)B(t_1)C(t_1)$. A similar procedure can be used to perform the averages of the terms with z^*_{1,t_1} and z_{2,t_1}, which are such that

$$\begin{aligned}
& \int d\mu(z_1) \int d\mu(z_2) z^*_{1,t_1} \langle \psi_0 \mid G^\dagger(0 z_1 | 0 t_1) A L G(z_1^* z_2 | t_1 t_2) B G(z_2^* 0 | t_2 0) \mid \psi_0 \rangle = \\
& \int_0^{t_1} d\tau \alpha^*(t_1 - \tau) \langle \Psi_0 | \left\{ V_{\tau - t_1} L^\dagger A L \right\} (t_1) B(t_2) | \Psi_0 \rangle ,
\end{aligned} \tag{9.12}$$

and

$$\begin{aligned}
& \int d\mu(z_1) \int d\mu(z_2) z^*_{1,t_1} \langle \psi_0 \mid G^\dagger(0 z_1 | 0 t_1) L^\dagger A G(z_1^* z_2 | t_1 t_2) B G(z_2^* 0 | t_2 0) \mid \psi_0 \rangle = \\
& \int_0^{t_2} d\tau \alpha(t_1 - \tau) \langle \Psi_0 | \left\{ A L^\dagger \right\} (t_1) \left\{ B V_{\tau - t_2} \right\} (t_2) | \Psi_0 \rangle .
\end{aligned} \tag{9.13}$$

Inserting (9.11), (9.12) and (9.13) in (9.5), we get the following equation for two-time correlations,

$$\begin{aligned}
& \frac{d}{dt_1} \langle \Psi_0 \mid A(t_1) B(t_2) \mid \Psi_0 \rangle = i \langle \Psi_0 \mid \{[H_S, A]\} (t_1) B(t_2) \mid \Psi_0 \rangle \\
+ \; & \int_0^{t_1} d\tau \alpha^*(t_1 - \tau) \langle \Psi_0 \mid \left\{ V_{\tau - t_1} L^\dagger [A, L] \right\} (t_1) B(t_2) \mid \Psi_0 \rangle \\
+ \; & \int_{t_2}^{t_1} d\tau \alpha(t_1 - \tau) \langle \Psi_0 \mid \left\{ [L^\dagger, A] V_{\tau - t_1} L \right\} (t_1) B(t_2) \mid \psi_0 \rangle \\
+ \; & \int_0^{t_2} d\tau \alpha(t_1 - \tau) \langle \Psi_0 \mid \left\{ [L^\dagger, A] \right\} (t_1) \left\{ B V_{\tau - t_2} L \right\} (t_2) \mid \Psi_0 \rangle + \mathcal{O}(g^3) .
\end{aligned} \tag{9.14}$$

Equations (9.14) represent the set of $\mathcal{Y}^2$ evolution equations for the correlation of system observables defined with a basis of $\mathcal{Y}$ operators. For a two-level system, $\mathcal{Y} = 3$, and the dimension of the operators in their matricial representation is 2.

In order to make use of equations (9.14) to calculate two time correlations, it is necessary to evolve initially the single mean value evolution equations up to time t. This is necessary since the initial value for the two time correlations is given by $\langle \Psi_0 \mid A(t_2)B(t_2) \mid \Psi_0\rangle = \langle \Psi_0 \mid C(t_2) \mid \Psi_0\rangle$, where $C = AB$.

The procedure followed in this section can be generalized to the computation of N-time correlation functions. Nevertheless, in the next section we propose a less involved method based on the hierarchy of equations, by which a general second order N-time correlation function is easier to obtain.

9.2.2 Computing second order MTCF with hierarchy of equations

We have shown in the Chapter (8) that the evolution of N-time correlation functions depends on $N+1$-time correlations when no approximations are made. Because of such dependency, some approximation has to be made in order to destroy the hierarchy and compute multiple time correlation function. Here the hierarchy is broken at the immediately higher level by using a second order perturbative approximation, first to the Schrödinger method described in Section (8.1), and second, to the Heisenberg method of Section (8.2), both of Chapter (8). It is shown that the evolution of two-time correlation functions is identical to that derived in the Section (9.2.1).

- Schrödinger formalism (Method I).

  The method of reduced propagators shown in Section (8.1) shows that the dependency on higher order correlations is due to the interaction (or coupling) between different propagators or trajectories. In particular, such coupling comes from the functional derivative, since it can be expressed as (8.15). The functional derivative appears in the dissipative term of the evolution equation of the propagators, and when averaging the noise term by using the properties (8.5) and (8.13). The coupling is avoided, and the hierarchy vanishes, when the functional derivative can be approximated as

$$\frac{\delta G(z_i^* z_{i+1}|t_i t_{i+1})}{\delta z_{i,\tau}^*} \approx O(z_{i+1} z_i^*, t_i, \tau) G(z_i^* z_{i+1}|t_i t_{i+1}), \tag{9.15}$$

  where $O(z_{i+1}z_i^*, t_i, \tau)$ is a system operator conveniently chosen for each case (see [41, 54, 40] for vacuum propagators, and [3, 4] for the general case $z_{i+1} \neq 0$). Although expression (9.15) is exact for some particular cases (i.e. when the interaction operator is diagonal $L \propto H_S$) (see for instance [3, 4, 40, 70]), generally some approximations have to be made in order to obtain $O(z_{i+1}z_i^*, t_i, \tau)$. Within the weak coupling approximation, a second order equation in the perturbative parameter g is obtained by only replacing O up to zero order in the evolution equations. The reason is that the term of the open equation (2.45) where the functional derivative appears, i.e. the dissipative term, is already of order g^2 due to the appearance of the two order correlation function $\alpha(t_i - \tau)$. Therefore, the term $\frac{\delta G(z_i^* z_{i+1}|t_i t_{i+1})}{\delta z_{i,\tau}^*} = \mathcal{M}_l \left[G(z_i^* z_l|t_i\tau) L G(z_l^* z_{i+1}|\tau t_{i+1})\right]$ up to order g^0 is,

$$\begin{aligned}
&\frac{\delta G(z_i^* z_{i+1}|t_i t_{i+1})}{\delta z_{i,\tau}^*} = \mathcal{M}_l \left[G(z_i^* z_l|t_i\tau) L G(z_l^* z_{i+1}|\tau t_{i+1})\right] \\
=\ & \langle z_i \mid \mathcal{U}_I(t_i\tau)\mathcal{U}_I^{-1}(t_i\tau)\mathcal{U}_I(t_i t_{i+1}) \mid z_{i+1}\rangle \\
=\ & V_{\tau - t_i} L G(z_i^* z_{i+1}|t_i t_{i+1}) + \mathcal{O}(g),
\end{aligned} \tag{9.16}$$

where $V_{\tau-t_i}L = \exp\left(iH_S(\tau-t_i)\right)L\exp\left(-iH_S(\tau-t_i)\right) = O(z_{i+1}z_i^*,t_i,\tau) \equiv O(t_i,\tau)$. Such time dependencies with the system Hamiltonian (denoted with V_{t_1}), are especially simple in the present case, since the operators are expressed in the system basis in which H_S is therefore diagonal.

Since this type of terms, which consists in a functional derivative inserted in an integral with $\alpha(t_i-\tau)$, also appear as a result of the analytical averages of the noise terms, following the properties (8.5) and (8.13), so that the same hypothesis can be made.

- Heisenberg formalism (Method II).

In the second method, the perturbative hypothesis is applied to the operators $L(\tau)$ which appears in equations (8.26), (8.32) and (8.35) when inserting the analytical solution of a_λ and $a_\lambda^\dagger$. The idea is to transform a two-time dependency on a one time-dependency [1], so that for instance,

$$\begin{aligned} & L^\dagger(\tau)\left\{[L,A]\right\}(t_i) = \mathcal{U}_I^{-1}(t_i0)L(\tau,t_i)[L,A]\mathcal{U}_I(t_i0) \\ = \; & \left\{V_{\tau-t_i}L^\dagger[L,A]\right\}(t_i) + \mathcal{O}(g), \end{aligned} \tag{9.17}$$

or

$$\begin{aligned} & L(\tau)B(t_{i+1}) = \mathcal{U}_I^{-1}(t_{i+1}0)L(\tau,t_{i+1})B\mathcal{U}_I(t_{i+1}0) \\ = \; & \left\{V_{\tau-t_{i+1}}LB\right\}(t_{i+1}) + \mathcal{O}(g). \end{aligned} \tag{9.18}$$

The perturbative equation for single time evolution is, up to second order,

$$\begin{aligned} & \frac{d}{dt_1}\langle\Psi_0 \mid A(t_1) \mid \psi_0\rangle = i\langle\Psi_0 \mid \left\{[H_S,A]\right\}(t_1) \mid \Psi_0\rangle\rangle \\ + \; & \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid \left\{V_{\tau-t_1}L^\dagger[A,L]\right\}(t_1) \mid \Psi_0\rangle \\ + \; & \int_0^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger,A]V_{\tau-t_1}L\right\} \mid \Psi_0\rangle. \end{aligned} \tag{9.19}$$

This equation is equal to the one obtained in [35, 41, 40, 54]. The two-time correlation equation (8.32) becomes, up to second order,

$$\begin{aligned} & \frac{d}{dt_1}\langle\Psi_0 \mid A(t_1)B(t_2) \mid \Psi_0\rangle = i\langle\Psi_0 \mid \left\{[H_S,A]\right\}(t_1)B(t_2) \mid \Psi_0\rangle \\ + \; & \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid \left\{V_{\tau-t_1}L^\dagger[A,L]\right\}(t_1)B(t_2) \mid \Psi_0\rangle \\ + \; & \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger,A]V_{\tau-t_1}L\right\}(t_1)B(t_2) \mid \psi_0\rangle \\ + \; & \int_0^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger,A]\right\}(t_1)\left\{BV_{\tau-t_2}L\right\}(t_2) \mid \Psi_0\rangle. \end{aligned} \tag{9.20}$$

This equation is equal to the one derived in the former section and in [3, 4, 2]. In those works the average over the terms in z_{i,t_i} is made by performing a perturbative expansion of the propagators, so that the properties

---

[1] We stress again that by time dependency we mean that related to the evolution operator $\mathcal{U}_I(t)$ with respec to the total Hamiltonian.

(8.5) and (8.13) are not needed. Applying the perturbative hypothesis in equation (8.35), we get the following equation for three time correlations up to second order in g,

$$\begin{aligned}
&\frac{d}{dt_1}\langle\Psi_0 \mid A(t_1)B(t_2)C(t_3) \mid \Psi_0\rangle = i\langle\Psi_0 \mid \{[H_S, A]\}\,(t_1)B(t_2)C(t_3) \mid \Psi_0\rangle \\
+&\int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid \left\{V_{\tau-t_1}L^\dagger[A, L]\right\}(t_1)B(t_2)C(t_3) \mid \Psi_0\rangle \\
+&\int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]V_{\tau-t_1}L\right\}(t_1)B(t_2)C(t_3) \mid \Psi_0\rangle \\
+&\int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]\right\}(t_1)\left\{B, V_{\tau-t_2}L\right\}(t_2)C(t_3) \mid \Psi_0\rangle \\
+&\int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{L^\dagger, A]\right\}(t_1)B(t_2)\left\{CV_{\tau-t_3}L\right\}(t_3) \mid \Psi_0\rangle. \qquad (9.21)
\end{aligned}$$

9.2.3 Generalization to a N-time correlation function

The second order evolution equations presented in the former sections can be generalized to N-time correlations. Such general equation is just the perturbative version of the equation (8.38). For that reason, in a similar way as in (8.38), we define a superoperator $\mathcal{P}_R$ that acts over the string $\{V_{\tau-t_1}L\}(t_1)\{A_2(t_2)\cdots A_N(t_N)\}$ in the following way:

$$\begin{aligned}
\mathcal{P}_R^0\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) &= \{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) \\
\mathcal{P}_R^1\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) &= A_2(t_2)\{V_{\tau-t_2}L\}(t_2)\hat{\mathbf{A}}^{(\mathbf{3})}(\hat{\mathbf{t}}^{(\mathbf{3})}), \\
\mathcal{P}_R^2\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) &= A_2(t_2)A_3(t_3)\{V_{\tau-t_3}L\}(t_3)\hat{\mathbf{A}}^{(\mathbf{4})}(\hat{\mathbf{t}}^{(\mathbf{4})}), \\
&\cdots \\
\mathcal{P}_R^{N-1}\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) &= \hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})})\{V_{\tau-t_N}L\}(t_N), \qquad (9.22)
\end{aligned}$$

and successively. Thus, the perturbative N-time correlation reads as follows,

$$\begin{aligned}
&\frac{dC_{\mathbf{A}}(\mathbf{t}|\Psi_0)}{d_t 1} = \langle\Psi_0 \mid [H_S(t_1), A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\
+&\int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid V_{\tau-t_1}L^\dagger(t_1)[A_1(t_1), L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\
+&\sum_{i=0}^{N-1}\int_{t_{i+2}}^{t_{i+1}} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid [L^\dagger(t_1), A_1(t_1)]\mathcal{P}_L^i V_{\tau-t_1}L(t_1)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle + \mathcal{O}(g^3).(9.23)
\end{aligned}$$

9.3 BEYOND THE QUANTUM REGRESSION THEOREM

We show in this section how non-Markovian multiple time correlation functions do not obey the Quantum Regression Theorem discussed in Section (7.2). This theorem, valid for Markovian interactions, states that the coefficients of the evolution of N-time correlation functions are the same as those for the single-time evolution,

$$\frac{d}{dt_1}\langle\Psi_0 \mid A(t_1) \mid \Psi_0\rangle \quad = \quad i\langle\Psi_0 \mid \{[H_S, A]\}\,(t_1) \mid \Psi_0\rangle\rangle$$

$$\begin{aligned} &+ \Gamma\langle\Psi_0 \mid \left\{L^\dagger[A,L]\right\}(t_1) \mid \Psi_0\rangle \\ &+ \Gamma\langle\Psi_0 \mid \left\{[L^\dagger,A]L\right\}(t_1) \mid \Psi_0\rangle + \mathcal{O}(g^3), \end{aligned} \tag{9.24}$$

where $\alpha(t_1-\tau) = \Gamma\delta(t_1-\tau)$. In the non-Markovian case, this evolution is given by

$$\begin{aligned} \frac{d}{dt_1}\langle\Psi_0 \mid A(t_1) \mid \Psi_0\rangle &= i\langle\Psi_0 \mid \{[H_S,A]\}(t_1) \mid \Psi_0\rangle \\ &+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid \left\{V_{\tau-t_1}L^\dagger[A,L]\right\}(t_1) \mid \Psi_0\rangle \\ &+ \int_0^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger,A]V_{\tau-t_1}L\right\}(t_1) \mid \Psi_0\rangle + \mathcal{O}(g^3). \end{aligned} \tag{9.25}$$

Since the equation for the N-time correlation function is given by (8.38) as

$$\begin{aligned} \frac{dC_{\mathbf{A}}(\mathbf{t}|\Psi_0)}{dt_1} &= \langle\Psi_0 \mid [H_S(t_1),A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\ &+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid L^\dagger(\tau)[A_1(t_1),L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\ &+ \sum_{i=0}^{N}\int_{t_{i+1}}^{t_i} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid [L^\dagger(t_1),A_1(t_1)]\mathcal{P}_R^{N-i}L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle, \end{aligned} \tag{9.26}$$

the coefficients are equal to those of (9.25) only if the operators are such that the displacement superoperator $\mathcal{P}_R$, that translate the operator $L(\tau)$ one place inside the string $\tilde{\mathbf{A}}(\tilde{\mathbf{t}})$, is such that

$$\mathcal{P}_R^{N-i}L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \equiv L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}), \tag{9.27}$$

a condition very difficult to fulfill. Moreover, let us now show the QRT does not held for non-Markovian interactions even within the weak coupling approximation. In order to do that, it is necessary to express in a different way the second order perturbative equations derived in the last section. Let us take for instance the two-time correlation function (9.14), and rearrange its last term as

$$\begin{aligned} &\int_0^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger,A]\right\}(t_1)\left\{BV_{\tau-t_2}L\right\}(t_2) \mid \Psi_0\rangle = \\ &\int_0^{t_2} d\tau\alpha(t_1-\tau)\langle\psi_0 \mid G^\dagger(0z_1|0t_1)\left\{[L^\dagger,A]\right\}\{[B,V_{\tau-t_2}L]\}(t_2) \mid \Psi_0\rangle \\ + &\int_0^{t_2} d\tau\alpha(t_1-\tau)\langle\psi_0 \mid G^\dagger(0z_1|0t_1)\left\{[L^\dagger,A]\right\}\{V_{\tau-t_2}LB\}(t_2) \mid \Psi_0\rangle \end{aligned} \tag{9.28}$$

Replacing this is (9.14), we get the following equation for second order two-time correlation,

$$\begin{aligned} &\frac{d}{dt_1}\langle\Psi_0 \mid A(t_1)B(t_2) \mid \Psi_0\rangle = i\langle\Psi_0 \mid \{[H_S,A]\}(t_1)B(t_2) \mid \Psi_0\rangle \\ + &\int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid \left\{V_{\tau-t_1}L^\dagger[A,L]\right\}(t_1)B(t_2) \mid \Psi_0\rangle \\ + &\int_0^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger,A]V_{\tau-t_1}L\right\}(t_1)B(t_2) \mid \psi_0\rangle \\ + &\int_0^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger,A]\right\}(t_1)\{[B,V_{\tau-t_2}L]\}(t_2) \mid \Psi_0\rangle + \mathcal{O}(g^3). \end{aligned} \tag{9.29}$$

The first three terms are analogous to the non-Markovian evolution of the quantum average of A from 0 to t_1 given by equation (9.25), so that only when the last term vanish, i.e. when $[L^\dagger, A] = 0$ or $[B, V_{\tau-t_2}L] = 0$, the Quantum Regression Theorem applies. Notice also that this term is zero in the Markovian case, since the corresponding correlation function $\alpha(t_1-\tau) = \Gamma\delta(t_1-\tau)$ is zero in the domain of integration from 0 to t_2.

Let us now take the perturbative equation for three time correlations (9.21), and manipulate its last two terms with a similar procedure. Thus

$$\begin{aligned} &+ \int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]\right\}(t_1)\left\{B, V_{\tau-t_2}L\right\}(t_2)C(t_3)\mid\Psi_0\rangle = \\ &+ \int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]\right\}(t_1)\left\{[B, V_{\tau-t_2}L]\right\}(t_2)C(t_3)\mid\Psi_0\rangle \\ &+ \int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]\right\}(t_1)\left\{V_{\tau-t_2}LB\right\}(t_2)C(t_3)\mid\Psi_0\rangle. \end{aligned} \tag{9.30}$$

For the last term of (9.21), we have

$$\begin{aligned} &\int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{L^\dagger, A]\right\}(t_1)B(t_2)\left\{CV_{\tau-t_3}L\right\}(t_3)\mid\Psi_0\rangle \\ =& \int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{L^\dagger, A]\right\}(t_1)B(t_2)\left\{[C, V_{\tau-t_3}L]\right\}(t_3)\mid\Psi_0\rangle \\ +& \int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{L^\dagger, A]\right\}(t_1)B(t_2)\left\{V_{\tau-t_3}LC\right\}(t_3)\mid\Psi_0\rangle. \end{aligned} \tag{9.31}$$

We now simplify the last term of (9.31)

$$\begin{aligned} &\int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{L^\dagger, A]\right\}(t_1)B(t_2)\left\{V_{\tau-t_3}LC\right\}(t_3)\mid\Psi_0\rangle = \\ &\int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid e^{iH_St_1}\left\{L^\dagger, A]\right\}e^{-iH_S(t_1-t_2)}Be^{-iH_S(t_2-t_3)} \\ &e^{-iH_S(\tau-t_3)}Le^{iH_S(\tau-t_3)}e^{iH_St_2}e^{-iH_St_2}Ce^{-iH_St_3}\mid\Psi_0\rangle + \mathcal{O}(g^3) \end{aligned} \tag{9.32}$$

where in the second line we have replaced the reduced propagators by their zero order in a perturbative expansion $G(t_it_{i+1}|z_i^*z_{i+1}) = \exp(z_i^*z_{i+1})\exp(-iH_S(t_i-t_{i+1}))$, and we have inserted the identity operator $1 = \exp(iH_St_2)\exp(-iH_St_2)$. Rearranging the terms we can express (9.32) as

$$\begin{aligned} &+ \int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{L^\dagger, A]\right\}(t_1)B(t_2)\left\{V_{\tau-t_3}LC\right\}(t_3)\mid\Psi_0\rangle = \\ &= \int_0^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{L^\dagger, A]\right\}(t_1)\left\{BV_{\tau-t_2}L\right\}(t_2)C(t_3)\mid\Psi_0\rangle + \mathcal{O}(g^3), \end{aligned} \tag{9.33}$$

which after reinsertion in (9.31), and then again in the equation (9.21), leads to the following expression

$$\begin{aligned} &\frac{d}{dt_1}\langle\Psi_0 \mid A(t_1)B(t_2)C(t_3)\mid\Psi_0\rangle = i\langle\Psi_0 \mid \left\{[H_S, A]\right\}(t_1)B(t_2)C(t_3)\mid\Psi_0\rangle \\ &+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid \left\{V_{\tau-t_1}L^\dagger[A, L]\right\}(t_1)B(t_2)C(t_3)\mid\Psi_0\rangle \end{aligned}$$

$$
\begin{aligned}
&+ \int_0^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]V_{\tau-t_1}L\right\}(t_1)B(t_2)C(t_3) \mid \Psi_0\rangle \\
&+ \int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]\right\}(t_1)\left\{[B, V_{\tau-t_2}L]\right\}(t_2)C(t_3) \mid \Psi_0\rangle \\
&+ \int_{t_4}^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]\right\}(t_1)B(t_2)\left\{[C, V_{\tau-t_3}L]\right\}(t_3) \mid \Psi_0\rangle \\
&+ \int_{t_4}^{t_3} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \left\{[L^\dagger, A]\right\}(t_1)\left\{[B, V_{\tau-t_2}L]\right\}(t_2)C(t_3) \mid \Psi_0\rangle + \mathcal{O}(g^3).
\end{aligned} \tag{9.34}
$$

Now the QRT is valid only when the last three terms are zero, which means that either $[L^\dagger, A] = 0$, or $[B, V_{\tau-t_2}L] = 0$ and $[C, V_{\tau-t_3}L] = 0$. The generalization to a perturbative equation of N-time correlation functions is straightforward, and has the following form,

$$
\begin{aligned}
&\frac{dC_{\mathbf{A}}(\mathbf{t}|\Psi_0)}{d_t1} = \langle\Psi_0 \mid [H_S(t_1), A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\
&+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid V_{\tau-t_1}L^\dagger(t_1)[A_1(t_1), L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\
&+ \int_0^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0[A_1(t_1), L(t_1)] \mid V_{\tau-t_1}L(t_1)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle \\
&+ \sum_{i=2}^{N}\int_{t_{i+1}}^{t_i} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid [L^\dagger(t_1), A_1(t_1)] \\
&\sum_{p=1}^{i-1}\mathcal{P}_R^p\left(\left\{[A_2, V_{\tau-t_2}L]\right\}(t_2)\tilde{\mathbf{A}}^{(\mathbf{3})}(\tilde{\mathbf{t}}^{(\mathbf{3})})\right) \mid \Psi_0\rangle.
\end{aligned} \tag{9.35}
$$

The superoperator $\mathcal{P}^p$ is defined in such a way that,

$$
\begin{aligned}
&\mathcal{P}^1\left(\left\{[A_2, V_{\tau-t_2}L]\right\}(t_2)\tilde{\mathbf{A}}^{(\mathbf{3})}(\tilde{\mathbf{t}}^{(\mathbf{3})})\right) = \left\{[A_2, V_{\tau-t_2}L]\right\}(t_2)\tilde{\mathbf{A}}^{(\mathbf{3})}(\tilde{\mathbf{t}}^{(\mathbf{3})}) \\
&\mathcal{P}^2\left(\left\{[A_2, V_{\tau-t_2}L]\right\}(t_2)\tilde{\mathbf{A}}^{(\mathbf{3})}(\tilde{\mathbf{t}}^{(\mathbf{3})})\right) = A_2(t_2)\left\{[A_3, V_{\tau-t_3}L]\right\}(t_3)\tilde{\mathbf{A}}^{(\mathbf{4})}(\tilde{\mathbf{t}}^{(\mathbf{4})}) \\
&\cdots
\end{aligned} \tag{9.36}
$$

$$
\begin{aligned}
&\mathcal{P}^{i-1}\left(\left\{[A_2, V_{\tau-t_2}L]\right\}(t_2)\tilde{\mathbf{A}}^{(\mathbf{3})}(\tilde{\mathbf{t}}^{(\mathbf{3})})\right) = \\
&A_2(t_2)\cdots A_{i-2}(t_{i-2})\left\{[A_{i-1}, V_{\tau-t_{i-1}}L]\right\}(t_{i-1})\tilde{\mathbf{A}}^{(\mathbf{i})}(\tilde{\mathbf{t}}^{(\mathbf{i})})
\end{aligned} \tag{9.37}
$$

The last integral of (9.35) corresponds to terms which are additional with respect to those appearing in the single time evolution, and therefore are responsible for the failure of the QRT in the non-Markovian limit. In consequence, the previous equations not only lead to the computation of the MTCF in the weak coupling limit, but they also express the conditions under which the QRT remain valid, i.e. that all the conmutators $[A_{i-1}, V_{\tau-t_{i-1}}L] = 0$ or that $[L^\dagger(t_1), A_1(t_1)] = 0$. Concerning this point, it is fundamental to notice that some correlations that formally obey the QRT might give rise to solutions from the equation (9.37) that differ from those given by the QRT. This happens in particular for those correlations that depend on others that do not obey the QRT.

9.4 EXAMPLES: APPLICATION OF THE STOCHASTIC METHOD AND THE SYSTEM OF EQUATIONS

9.4.1 A solvable example

To illustrate the theory proposed in this chapter, we shall apply it to a simple solvable model. Consider the Hamiltonian (7.40) with $H_S = \frac{\omega_S}{2}\sigma_z$ and $L = \sigma_z$. This model describes the dynamics of system state vectors towards one of the eigenstates of the system Hamiltonian. It turns out that because $[H_S, L] = 0$, then $O = L$ in equation (7.50). We have shown in Section (5.3.1) that the reduced propagator is diagonal and it is explicitly given by

$$
\begin{aligned}
G(z_1^* z_2|t_1 t_2) = \exp\Big\{ & -i\frac{\omega_S}{2}(t_1 - t_2)\sigma_z + L\int_{t_2}^{t_1} d\tau z_{1,\tau}^* - L^\dagger \int_{t_2}^{t_1} d\tau z_{2,\tau}^* \\
- \quad & LL^\dagger \int_{t_2}^{t_1} d\tau \int_{t_2}^{\tau} ds\alpha(\tau - s) + z_1^* z_2 \Big\}. \qquad (9.38)
\end{aligned}
$$

We first look at the expectation values of system observables, since they will be useful in our discussion. Let us consider an observable A that has, in the basis of eigenvectors of σ_z, the matrix representation $A = \{\{0, \alpha\}, \{\beta, 0\}\}$. For an initial state $|\Psi_0\rangle = |\psi_0\rangle|0\rangle$, the expectation value of A is formally given by

$$
\langle A\rangle = M\big[\langle\psi_0|G^\dagger(0z|0t_2)AG(z^*0|t0)|\psi_0\rangle\big]. \qquad (9.39)
$$

From equations (9.38) and (9.39), performing the average over the environment degrees of freedom it is obtained,

$$
\langle A\rangle = e^{-2\int_0^t d\tau \int_0^\tau ds(\alpha(\tau - s) + \alpha^*(\tau - s))}\big\{\alpha\langle\psi_{01} \mid \psi_{01}\rangle e^{i\omega_S t} + \langle\psi_{02} \mid \psi_{02}\rangle e^{-i\omega_S t}\big\},
$$

where we have taken a normalized initial system state $|\psi_0\rangle =| \psi_{01}\rangle+ | \psi_{02}\rangle$. In the same manner, it follows for $\langle\sigma_z\rangle$

$$
\langle\sigma_z\rangle = \langle\psi_{01} \mid \psi_{01}\rangle - \langle\psi_{02} \mid \psi_{02}\rangle.
$$

Now we turn our attention to the multiple-time correlation functions. We shall compute in particular the $two - time$ correlations, whereas higher order time correlations can be treated in the same vein and they do not introduce any new consideration. In this regard the two-time correlation functions contain all the necessary and not trivial ingredients that enter in the computation of higher order correlation functions. Let us consider the observables $A = \{\{0, \alpha\}, \{\beta, 0\}\}$, $B = \{\{1, 0\}, \{-1, 0\}\} = \sigma_z$, and their two-time correlation function (7.44) is

$$
C_{AB}(t_1 t_2|\Psi_0) = M_{1,2}\big[\langle\psi_0|G^\dagger(0z_1|0t_1)AG(z_1^* z_2|t_1 t_2)BG(z_2^* 0|t_2 0)|\psi_0\rangle\big]. \qquad (9.40)
$$

If we insert the equation (9.38) into (9.40) the following expression is obtained

$$
C_{AB}(t_1 t_2|\Psi_0) = e^{-2\int_0^{t_1} d\tau \int_0^{t_1} ds\alpha(\tau - s)}\big\{ - \alpha\langle\psi_{01} \mid \psi_{02}\rangle e^{i\omega_S t_1} + \beta\langle\psi_{02} \mid \psi_{01}\rangle e^{-i\omega_S t_1}\big\}. \qquad (9.41)
$$

As in the previous cases, once the environment correlation function is known, the time correlation function can be directly computed. In the case in which $A = B = \sigma_z$, we have $C_{\sigma_z\sigma_z} = 0$.

Let us now calculate the evolution equations for the two-time correlation functions and investigate their relation to the QRT. To this purpose, we first consider the time derivative of the mean averages $\langle\sigma_i\rangle, i =$

(x, y, z) from the general form (9.39), which results in the following set of coupled linear differential equations

$$\begin{aligned}
\frac{\partial\langle\sigma_x\rangle}{\partial t} &= \quad -D(t)\langle\sigma_x\rangle - \omega_S\langle\sigma_y\rangle \\
\frac{\partial\langle\sigma_y\rangle}{\partial t} &= \quad -D(t)\langle\sigma_y\rangle + \omega_S\langle\sigma_x\rangle \\
\frac{\partial\langle\sigma_z\rangle}{\partial t} &= \quad 0,
\end{aligned}$$

with

$$D(t) = 2\int_0^t d\tau(\alpha(t-\tau) + \alpha^*(t-\tau)). \tag{9.42}$$

In the same manner, the following set of equations for the two-time correlation functions is obtained by deriving the equation (9.41),

$$\begin{aligned}
\frac{C_{\sigma_x\sigma_z}}{\partial t_1} &= \quad -D(t_1)C_{\sigma_x\sigma_z} - \omega_S C_{\sigma_y\sigma_z} \\
\frac{C_{\sigma_y\sigma_z}}{\partial t_1} &= \quad -D(t_1)C_{\sigma_y\sigma_z} + \omega_S C_{\sigma_y\sigma_z} \\
\frac{C_{\sigma_z\sigma_z}}{\partial t_1} &= \quad 0.
\end{aligned}$$

Comparing the equations (9.42) with the equations (9.43), we could draw the tentative conclusion that the QRT is valid for this model. However, as discussed in the previous sections, the validity of the QRT follows from the fact that in this case we have $[V_{\tau-t}L, B] = 0$, and therefore the last term of equation (9.14) is zero. To illustrate that the validity of the QRT can not be considered general, we study an example in which neither $[L, B] = 0$ nor $[L^\dagger, A] = 0$: the time correlation $C_{\sigma_x\sigma_y}(t_1t_2)$. We start by considering the general anti-diagonal system operators $A = \{\{0, \alpha\}, \{\beta, 0\}\}$ and $B = \{\{0, \alpha'\}, \{\beta', 0\}\}$. The analytical derivation of their two-time correlation function leads to

$$C_{AB}(t_1t_2) = e^{\tilde{D}(t_1t_2)}\{\alpha\beta'\langle\psi_{01} \mid \psi_{01}\rangle e^{i\omega_S(t_1-t_2)} + \alpha'\beta\langle\psi_{02} \mid \psi_{02}\rangle e^{-i\omega_S(t_1-t_2)}\}, \tag{9.43}$$

where we have defined

$$\begin{aligned}
\tilde{D}(t_1t_2) = &\int_0^{t_1} d\tau \int_0^{\tau} ds\,\alpha^*(\tau-s) + \int_{t_2}^{t_1} d\tau \int_t^{\tau} ds\,\alpha(\tau-s) \\
&+ \int_0^{t_2} d\tau \int_0^{\tau} ds\,\alpha(\tau-s) + \int_0^{t_1} d\tau \int_t^{t_1} ds\,\alpha(\tau-s) \\
&- \int_{t_2}^{t_1} d\tau \int_0^{t_2} ds\,\alpha(\tau-s) - \int_0^{t_1} d\tau \int_0^{t_2} ds\,\alpha(\tau-s).
\end{aligned}$$

For the case of $C_{\sigma_x\sigma_y}(t_1t_2)$, on the one hand we have

$$C_{\sigma_x\sigma_y}(t_1t_2) = e^{-\tilde{D}(t_1t_2)}\{i\langle\psi_{01} \mid \psi_{01}\rangle e^{i\omega_S(t_1-t_2)} - i\langle\psi_{02} \mid \psi_{02}\rangle e^{-i\omega_S(t_1-t_2)}\}, \tag{9.44}$$

and on the other hand its derivative with respect to t_1

$$\frac{\partial C_{\sigma_x\sigma_y}(t_1t_2)}{\partial t_1} = \frac{\partial\tilde{D}(t_1t_2)}{\partial t_1}C_{\sigma_x\sigma_y}(t_1t_2) - \omega_S C_{\sigma_x\sigma_x}(t_1t_2). \tag{9.45}$$

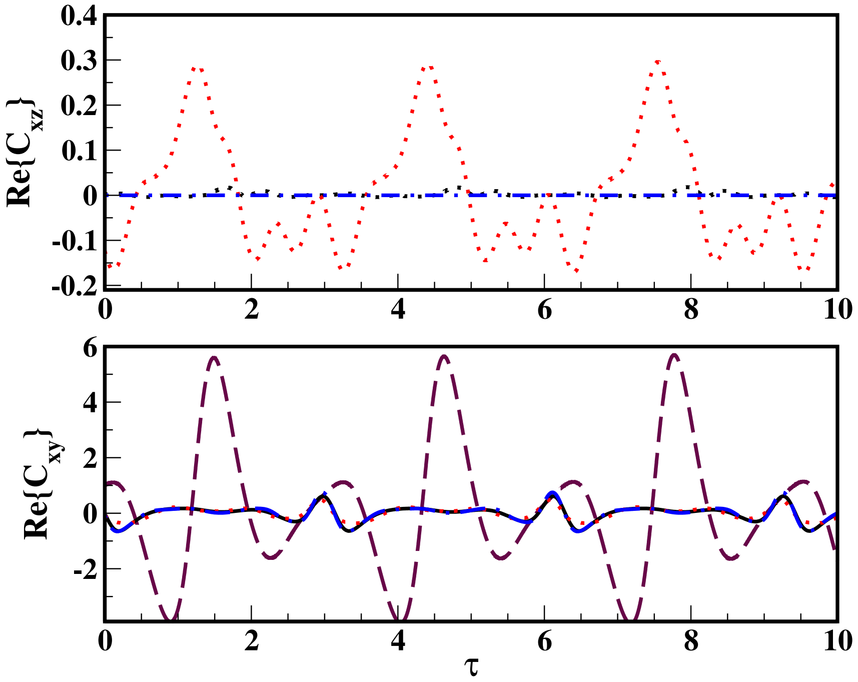

Fig. 9.2 In the figure different two-time correlation functions are displayed. The upper figure corresponds to the real part of $C_{\sigma_x\sigma_z}$ and the lower to the real part of $C_{\sigma_x\sigma_y}$. In the upper figure, the solid line corresponds to the analytical result (9.41) that in *this case* coincides with the result expected from the Quantum Regression Theorem. The dot-dashed line is the result of an average over 10^2 trajectories and the dotted line to an average over 10^5 trajectories. In the lower figure, the long-dashed line is the result given by the QRT. Compared to the exact result given by (9.43) (solid line), clearly the QRT is not valid for $C_{\sigma_x\sigma_y}$. The dot-dashed and dotted lines are the result of and average over 10^2 and 10^4 trajectories respectively.

We can see from this last equation that the time derivative of the correlation function $C_{\sigma_x\sigma_y}$ does not satisfy the Quantum Regression Theorem, a result that illustrates the conclusion drawn in the previous section and the fact that the theory here introduced applies for both Markovian and non-Markovian cases. Equation (9.45) have been computed by deriving the exact solution (9.44), but it can also be obtained from the general equation (9.14). Although this last equation is derived under the weak coupling assumption, it is also valid for the present model, since the expression $O = L$ is also obtained under a perturbative expansion of the operator.

Figures 9.2 and 9.3 show respectively the real and imaginary parts of two-time correlation functions of the system (7.40), $C_{\sigma_x\sigma_z}$ and $C_{\sigma_x\sigma_y}$. The exact result (9.44) is compared to the one obtained through the stochastic propagators as explained in Section 9.1. When the number of trajectories in the stochastic ensemble is large enough, both results are the same, which proves the validity of the stochastic method. The number of oscillators of the environment have been set equal to two. The parameters used were $g_1, g_2 = g = 1$ and $\omega_1 = 6, \omega_2 = 2$. The initial system state taken was $|\Psi_0\rangle =| \psi_0\rangle|00\rangle$ with $|\psi_{01}\rangle = \frac{1+2i}{\sqrt{7}} \mid +\rangle$ and $|\psi_{02}\rangle = \frac{1+i}{\sqrt{7}} \mid -\rangle$. It is also clear from the figures that the QRT does not apply for $C_{\sigma_x\sigma_y}$, since $[V_{\tau-t}L, B] \neq 0$ and $[L^\dagger, A] \neq 0$.

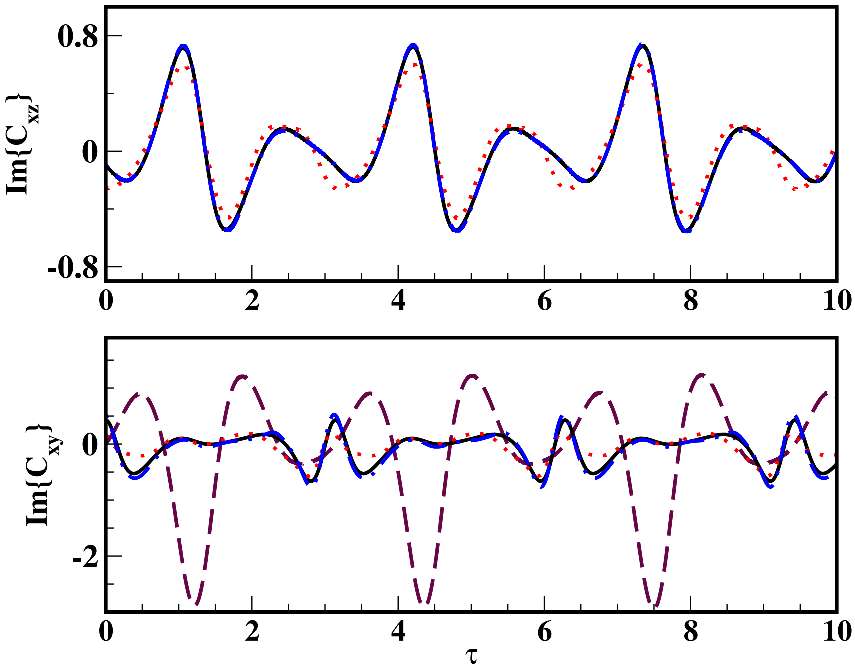

Fig. 9.3 The figure displays the same as figure 9.2, but now for the imaginary parts of $C_{\sigma_x\sigma_z}$ and $C_{\sigma_x\sigma_y}$. In the upper figure, again the analytical result (9.41) coincides with the result expected from the Quantum Regression Theorem (both in solid line). Dot-dashed and dotted line corresponds to the result of an average over 10^2 and 10^5 trajectories respectively. In the lower figure, the analytical result (solid line) differs from that given by the QRT (long-dashed). The dot-dashed and the dot lines are the result of and average over 10^2 and 10^4 trajectories respectively.

9.4.2 An example of dissipative system within the weak coupling limit

Let us now compute two time correlations for a two level system with $H_S = \frac{\omega_S}{2}\sigma_z$ with a dissipative interaction with $L = \sigma_{12}$. Within the perturbative approximation, the operator $\bar{O}(z_{i+1}z_i^*, t_i, \tau)$ can be replaced by its zero order perturbative expansion, $V_{\tau-t}L = \sigma_{12}\exp\{i\omega_S(t-\tau)\}$, where ω_S is the system rotating frequency. Like in Section (5.3.2), we propose the following *approximated* correlation function,

$$\alpha^{apprx}(t-\tau) = \sum_{m=-\nu/2}^{\nu/2} C(m)e^{-i\pi m(t-\tau)/T_{max}}, \tag{9.46}$$

with the coefficients

$$C(m) = \frac{1}{2T_{max}}\int_{-T_{max}}^{T_{max}} dt\alpha(t)e^{i\pi mt/T_{max}}. \tag{9.47}$$

which represents the Fourier series for the function $\alpha(t-\tau) = (\Gamma/2)\exp\{\Gamma|t-\tau|\}$. The quantity T_{max} is again the time window in which the correlation function is expanded in the series. The more members we add in the former sum, the closer is the solution to the exponential decaying correlation function, and the larger we can fix the the recurrence time T_{max}. However, it is observed that for only $\nu = 8$ oscillators, we can already choose parameters (g, Γ, and the environmental correlation time τ_c) such that the second order two-time correlations present a decaying behavior (i.e. dissipation) before the recurrence time.

We choose $t_2 = 1$, $g = 0.5$ and $\Gamma = 1$, so that the decaying behavior can be already observed at short times (up to $t_1 - t_2 = \tau = 50$). In figure (9.4), we represent the correlation $C_{\sigma_x\sigma_x}$, comparing the result of the evolution equation (9.14) to the ensemble averaged stochastic evolution, given by equation (7.44) for different number of trajectories. The last result is obtained by following the steps described in Section (9.1).

Let us now consider a very large number of oscillators composing the sum (9.46), i.e. the correlation function $\alpha(t-\tau) = (\Gamma/2)\exp\{-\Gamma|t-\tau|\}$, in order to study the validity of the QRT for the $C_{\sigma_x\sigma_x}$. This is a typical case in which the last term of (9.14) does not vanish, so that the result of the QRT differ to the one of (9.14), as displayed in Figure. (9.5).

9.4.3 Spin-boson model

We now apply the equations derived in this paper to the problem of a spin coupled to a thermal reservoir, as described by [37, 35]. We consider the Hamiltonian (7.40) with $H_S = \frac{\omega}{2}\sigma_z$, a coupling operator $L = \sigma_x$, and an interaction Hamiltonian with magnitude small enough as to be considered perturbative. Within this model, the bath can be characterized by the spectral strength given by (5.110),

$$J(\omega) = \frac{\omega^3}{\omega_c^2}e^{-\omega/\omega_c}, \tag{9.48}$$

where ω_c is a cutoff frequency [35, 37], here chosen as $\omega_c = 1$. The correlation function of the noise generated by a thermal bath and where $L = L^\dagger$ is given in terms of $J(\omega)$ as (see Appendix (L) for a derivation of such correlation in the case of thermal two-time correlation functions with $L = L^\dagger$.),

$$\alpha(t) = \int_0^\infty d\omega J(\omega)\left[\coth\left(\frac{\omega\beta}{2}\right)\cos(\omega t) - i\sin(\omega t)\right]. \tag{9.49}$$

The inverse temperature $\beta = (k_B T)^{-1}$ is chosen according to the energy of the bath, and considering that the energy of the subsystem is very small compared to it [37, 35].

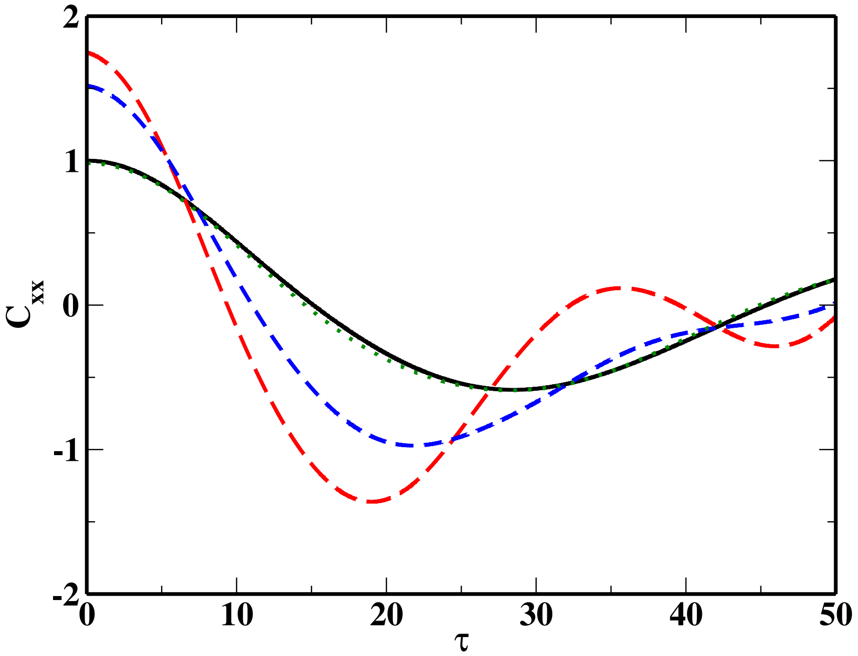

Fig. 9.4 Two time correlation $C_{xx} = C_{\sigma_x \sigma_x}$ for the coupling $L = \sigma_{12}$, and the dissipative Fourier series of the exponential correlation function with $\nu = 8$ oscillators. The initial condition chosen is the same as in the former figure, $|\psi_0\rangle = \big((1+2i)|+\rangle + (1+i)|-\rangle\big)/\sqrt{7}$, and the parameters are: $\omega_S = 0.1$, $\Gamma = 1$, perturbative parameter $g = 0.2$, recurrence time $T_{max} = 40$, and initial time for the correlation $t_2 = 1$. Solid line represents the solution of the system (9.14), whereas long-dashed, dot-dashed, and dotted lines gives the result of the stochastic method for $\kappa = 50 \times 10^4$, $\kappa = 10^5$ and 10^7 trajectories respectively. An increasing accordance with the system curve is observed, as the number of trajectories grows.

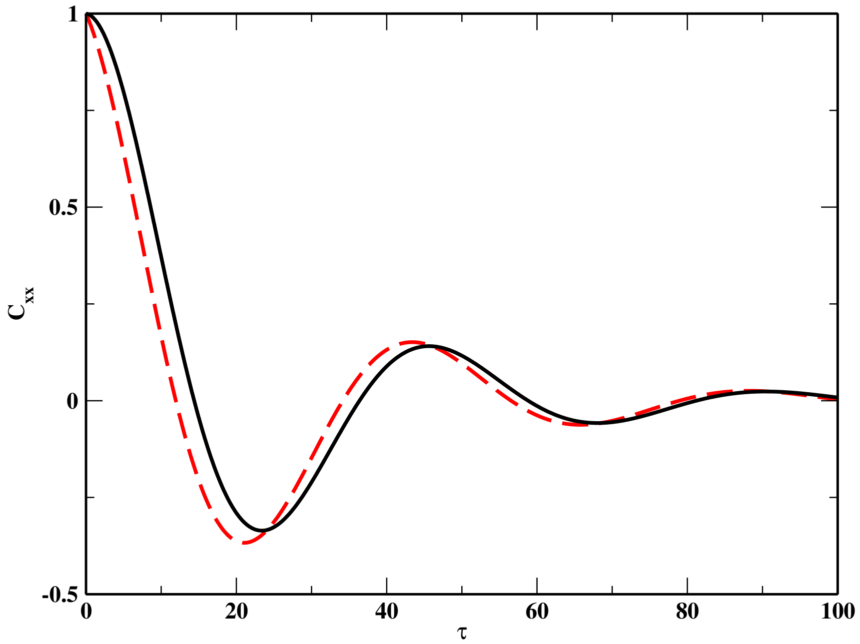

Fig. 9.5 Two time correlation $C_{xx} = C_{\sigma_x \sigma_x}$ for the coupling $L = \sigma_{12}$, and the dissipative correlation function $\alpha(t-\tau) = -(\Gamma/2)\exp\{-\Gamma|t-\tau|\}$. The initial condition chosen is the same as in the former figure, and the parameters are: $\omega_S = 0.1$, $\Gamma = 1$, perturbative parameter $g = 0.4$, and initial time for the correlation $t_2 = 10$. Solid line represents the solution of the system (9.14), and long-dashed line gives the result expected with the QRT. Because the last term in (9.14) is non zero, both results are different from each other, and the QRT is not valid.

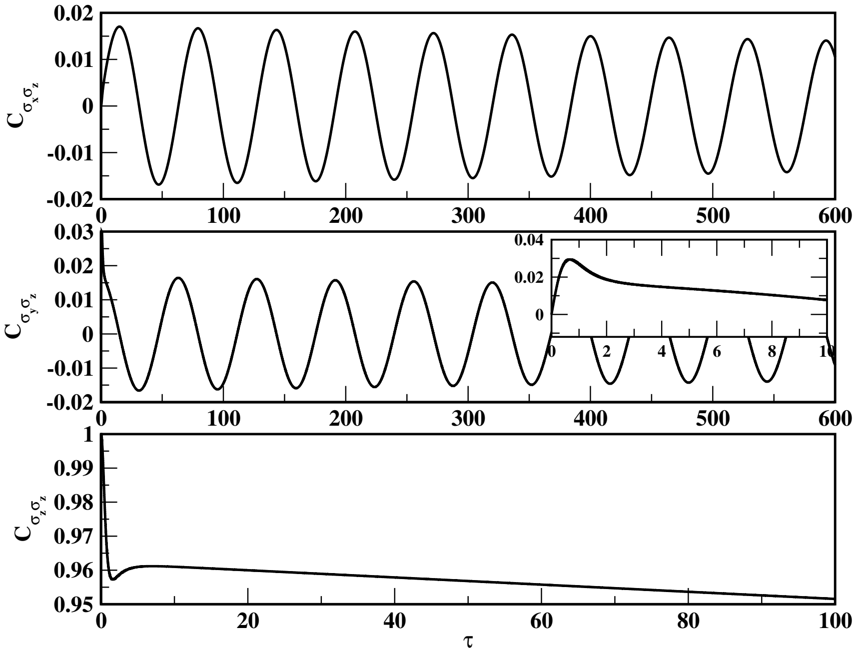

Fig. 9.6 The figure displays some two-time correlation functions for the spin-boson model within the perturbative approximation and for $\beta = 10$. In the long time limit $C_{\sigma_i,\sigma_j} \equiv \langle\sigma_i\rangle\langle\sigma_j\rangle$, for $i, j = x, y, z$. At this low temperature, a strong oscillatory behavior due to the mean values $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ is observed in the corresponding two-time correlations, which in the long term is damped by the dissipation caused by $\langle\sigma_z\rangle$. With this reasoning, it can be easely infered why the last correlation, $C_{\sigma_z\sigma_z}$, only presens a dissipative behavior. Some non-Markovian structure of the short time dynamics is displayed in the caption.

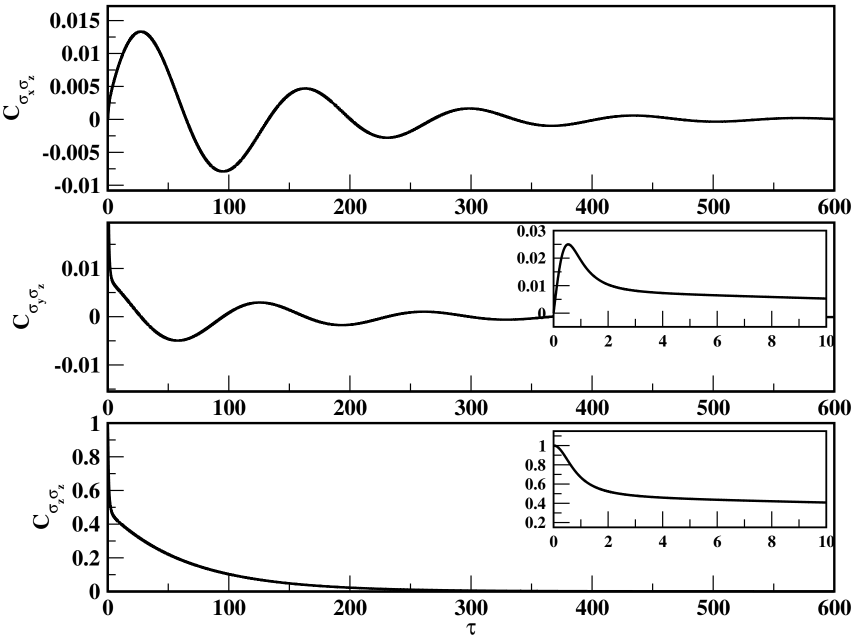

Fig. 9.7 The figure displays some two time correlation functions for the spin-boson model within the perturbative approximation and for $\beta = 0.1$. For high temperatures the dissipation becomes much more efficient than for lower temperatures (see Fig.(9.6)), and the oscillatory behavior is strongly damped in $C_{\sigma_x\sigma_z}$ and $C_{\sigma_y\sigma_z}$. Moreover, the correlation $C_{\sigma_z\sigma_z}$ decays much faster than in the low temperature case. Again, some non-Markovian structures of the short time dynamics are displayed in the captions.

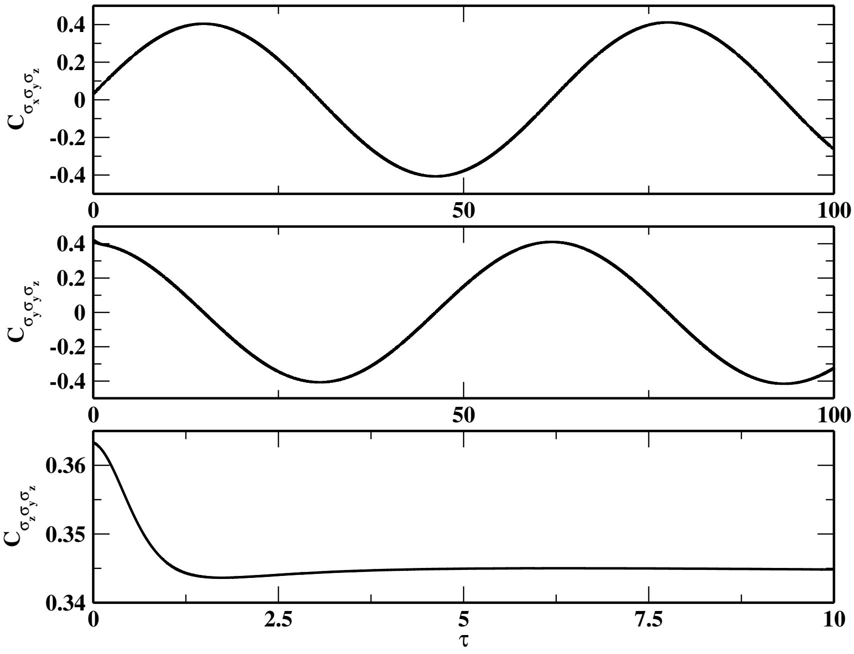

Fig. 9.8 Some three-time correlation function of the spin-boson model are displayed within the perturbative approximation and for $\beta = 10$.

10

Conclusions of this part

We formulate in this part of the thesis a theory of non-Markovian multiple-time correlations functions (MTCF) with the use of the reduced propagators derived in Chapter (2). The results are discussed throughout three different chapters.

- In Chapter (8) a hierarchy of equations is derived that formaly obey non-Markovian MTCF. This hierarchy shows how in general N-time correlation functions depend on $N+1$-time correlations.
- In Chapter (9) the weak coupling approximation is used to derive the system of equations that evolve MTCF up to second order in the perturbative parameter g. With such approximation, the hierarchy is destroyed, and N-time correlations only depend on other N-time correlations, as well as on $N-1$-time correlations to set up their initial conditions. The resulting equations are therefore suitable for computational purposes. Having the evolution equations of MTCFs we show the failure of the Quantum Regression theorem in non-Markovian interactions. This theorem states that the evolution of N-time correlations is given by the same equation as single-time correlations, i.e. by the master equation. In the non-Markovian equations we propose, several new terms appear with respect to those of the equation of single-time correlations.

  In this chapter, a stochastic method to compute MTCFs is also proposed, which consists in performing a sampling of different trajectories of the reduced propagator by considering z_{i+1,t_i} and z_{i,t_i} as Gaussian noises. The second order MTCFs obtained with the stochastic sampling and with the system of equations above derived are equal to each other. This is illustrated by applying both methods to three different systems: a solvable model with $L \propto H_S$, a system that interacts with the bath with exponentially decaying correlation function and through a non diagonal coupling, and a spin-boson model.

Part IV

DYNAMICS OF A TWO LEVEL SYSTEM IN A PBG MATERIAL

As noted in the introduction, one of the most interesting examples of non-Markovian interaction is that of an atom coupled to a radiation field within a PBG material. In this part of the thesis we are interested in applying some of the dynamical equations developed in Parts (II) and (III) to such a system. The study is divided in two chapters,

- In Chapter (11) a model to describe the system is generated. The Hamiltonian of a two level atom in contact with a radiation field, as well as the dependencies of the coupling constants g_λ, were already obtained in Chapter (1). It was also shown that the **correlation function** $\alpha(t-\tau)$ can be constructed with the knowledge of such constants and the frequencies ω_λ. Among other factors, the g_λ depend on the dispersion relation of the field. In this chapter, we propose a model for the dispersion relation of the radiation field within a PBG, and follow the microscopic derivation of Section (1.3.1.1) to generate the $\alpha(t-\tau)$ characteristic of such field. As we have seen throughout this work, such a function is very important, since it enters in all the dynamical equations that evolve either quantum mean values or MTCF of a QOS.

  Several correlation functions in time have previously been proposed in the literature [42]. However, they are singular at the origin, which makes them unsuitable to **generate a noise** z_t such that $\mathcal{M}[z_t z_\tau^*] = \alpha(t-\tau)$. The correlation function we propose captures many of the physically relevant aspects of the problem and describes the short time behavior in a more accurate way than previously proposed ones [42]. In addition, it does not have a singularity at the origin. This permits a correct description of the fluctuations of the EM field, i.e. the noise in the stochastic formalism, and a better description of the non-Markovian effects in the atomic dynamics. Further details of such new correlation function and its derivation can be found in Appendix (N).

- In Chapter (12) we study the dynamics of **expectation values** by using non-Markovian stochastic Schrödinger equations. In order to check its validity, we shall study several of the physical phenomena occurring in atoms within a PBG material, that have been already described in literature within non-Markovian master equations, such as the long time limit residual population in the excited level of the atom and the population inversion which occurs in the atomic system when applying an external laser field [42]. In addition to the stochastic equation, we study the two second order perturbative master equations presented in Chapter (5): the non convoluted and the convoluted equations. We show that this last equation, which is the one used in previous studies of the system [42], does not preserve positivity for certain parameter values, while the non convoluted equation preserves positivity by construction.

Finally, in Section (12.4) we study some **fluctuations** of the two level atom. As argued in Chapter (III), this result may be useful in the future to compute its emission spectra. Four-time correlation functions can also be calculated in the same way and used to compute joint-emission probabilities. Hence, this particular issue remains open and full of interest for future work.

The formulation we present here can be extended to the study of more complex systems, such as many level atoms embedded in more complicated band gap structures. This is interesting since, as noted before the stochastic scheme becomes computationally more efficient than master equations when the number of degrees of freedom of the system increases.

Several conclusions of this part of the thesis are drawn in Chapter (13).

11

The model

11.1 PHOTONIC CRYSTALS.

When light enters into a medium with a different refraction index, it may be scattered into a reflected and a refracted part. While the reflected light is scattered back to the initial medium, the refracted light enters through the new medium suffering a change of velocity, which produces a variation in its direction of propagation. The light traversing a homogeneous medium which has the same refraction index in all directions is not scattered.

Suppose that we have a material where the refraction index changes in one direction. Then, only the light entering in such direction may be scattered (refracted and reflected). If we now consider this change in the refraction index to be periodical, then the scattering process will be repeated every time the light suffers a new change in the refraction index. This can be achieved by constructing a crystal with alternating layers of width b and a high refraction index n_r, with layers of low refraction index (which for simplicity is considered the unity), in such a way that they are separated by a length a. Thanks to the periodicity, the rays are scattered coherently, allowing some of them to interfere. A maximum in the reflection is formed when the reflected rays interfere constructively, which occurs when the Bragg condition is verified [110]. For rays entering perpendicularly to the layers (i.e. in the direction of change of the refraction index), such condition is given by

$$2a = \lambda_0, \tag{11.1}$$

with λ_0 the vacuum wavelength. The rays of light entering perpendicularly to the layers and with wavelength given by the former relation are scattered back (or reflected) and do not appear in the crystal. This gives rise to the formation of a forbidden band or a gap within the material corresponding to those modes. In this example, the gap is one-dimensional, since it only appears for modes corresponding to the scattering direction [1].

---

[1] In addition to the Bragg effect, there are certain wavelengths giving rise to a maximum in the reflection coefficient from a single layer. This maximum, known as Mie resonance [119, 46], occurs for $\lambda/4n_r = 2b$. The combination of these two conditions yields to the

This kind of crystals are known as Photonic Band Gap (PBG) materials (also photonic crystals (PC)), and were first proposed by John and Yablonovitch [13, 12, 111] a means to localize and trap light in a bulk material [13], and to produce a complete inhibition of spontaneous emission over a broad frequency range [12].

Following a procedure analogous to the above described, a $3D$ gap can be fabricated by generating a three dimensional dielectric periodic structure. In that case, the light incident in the material with a frequency related with the lattice constant will be backscattered from the material, independently of the angle of incidence.

Another way to understand the band gap structure of a PC is by considering them as the optical analogs of semiconductor crystals for electrons. Instead of a periodically ordered array of atoms which scatters the electrons and modifies their energy-momentum relation, PC are composed of a periodic dielectric lattice, in such a way that the refraction index is spatially periodic. In semiconductor crystals, the eigensolutions of the electron in the periodic potential differs from that in the absence of the potential, and for certain eigenvalues there are no corresponding eigensolutions. In the same way, within a PC there are certain frequency values ω for which there is no corresponding wave vector or field mode $\mathbf{k}$. Thus, the relation between both magnitudes (also known as dispersion relation) presents a special structure in which the bands of permitted frequencies (for which there are propagating photon modes), are separated by gap regions of forbidden values of ω.

The band gap structure can also be viewed in the photonic density of states of the radiation field, which presents frequency regions in which it is different from zero, corresponding to the bands, and regions in which it vanishes, corresponding to the gaps. Additionally the photon density of states varies rapidly near the edge of the gap, which implies that the correlation time of the vacuum fluctuations is not negligibly small on the time scale of evolution of an atomic system. This fact makes inappropriate the usual Markovian approximation applied in quantum optics in the treatment of the interaction of atoms with electromagnetic radiation. The dynamics of an excited atom with resonant frequency near the edge of a gap presents some particular features, including the inhibition of spontaneous emission [112], the strong localization of light [13], the formation of atom-photon bound states [113] and the atomic inversion in the steady state [114].

PBG materials have attracted considerable attention in the scientific and engineering community because of their many potential possibilities and applications. In that sense, the literature about PC is so large that an exhaustive review is out of the scope of this thesis (instead, we shall refer the reader to [46] for a good review). In this work, we are concerned about giving a theoretical description of the some of the dynamical aspects of a two level atom inside a PBG. This includes a description of some of the effects above mentioned. Hence, this introduction, combined with the description of the model we offer in the next sections is sufficient for our purpose.

11.2 TWO LEVEL SYSTEM IN A PBG

In the last chapters, we have established a second order master equation, a second order stochastic Schrödinger equation, and a set of second order MTCFs valid for describing the dynamics of any quantum open system in contact with a non-Markovian harmonic oscillator reservoir described by a linear coupling Hamiltonian.

In this section, we will be concerned with the study of a quantum open system with two levels (a two level atom) interacting with an electromagnetic field or reservoir immersed in the photonic crystal. We follow the description introduced in Section (1.2) for a general atom-electromagnetic field interaction, particularizing the discussion for the PBG radiation field.

optimal relation between the lattice constant, a, and the microscopical elements (in this case dielectric layers) with dimension b, to produce a wide gap. This combination is $2b/a = 1/2n_r$.

The atom-radiation Hamiltonian is well known to have the form [43]:

$$H_{tot} = \frac{1}{2m_e}[\mathbf{p} - e\mathbf{A}(\mathbf{r})]^2 - e\Phi(\mathbf{r}) + \sum_\lambda w_\lambda a_\lambda^\dagger a_\lambda, \tag{11.2}$$

where $\mathbf{p}$ and m_e represent the momentum and mass of the atomic transition electron, and $\mathbf{A}(\mathbf{r})$ and $\Phi(\mathbf{r})$ are the electromagnetic vector and scalar potential. In the basis of non-perturbed wave functions of the system, the Hamiltonian H_S for a two level system is

$$H_S = \frac{\omega_S}{2}(\sigma_{22} - \sigma_{11}), \tag{11.3}$$

where ω_S is the transition frequency between the two atomic levels and $\sigma_{ij} = |i\rangle\langle j|$ are the atomic pseudospin operators. An interaction Hamiltonian of the form $\sum_\lambda g_\lambda(a_\lambda^\dagger L + L^\dagger a_\lambda)$ is obtained by assuming the electric dipole approximation in (11.2). This approximation is justified by considering that the atom is small in comparison with the size of the unit cell of the PC [115]. In that case, the atom experimenting electronic transitions between levels interacts with the field as an oscillatory dipole. The approximation involves therefore not considering in (11.2) the term $\mathbf{A}(\mathbf{r})^2$, which involves processes of more than one photon.
In general, the mode functions $\mathbf{A}(\mathbf{r})$ may be expanded in any complete set of basis functions spanning the region under consideration. In free space the usual choice is a basis of plane waves, whereas in a photonic crystal a periodic basis of Bloch modes [144] satisfying the Bloch-Floquet theorem [106]

$$\mathbf{A}_\mathbf{k}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\mathbf{A}_\mathbf{k}(\mathbf{r}), \tag{11.4}$$

is more convenient, since it permits taking advantage of the optical periodicity of the field. For the case of a two level atom studied the coupling strengths g_λ become

$$g_\lambda = \omega_S d_{21}[\frac{1}{2\epsilon_0\omega_\lambda v}]^{\frac{1}{2}} \mathbf{e}_\lambda \cdot \mathbf{u_d}, \tag{11.5}$$

where ω_λ is the frequency of the mode λ [42]. The vectors $e_\lambda \equiv e_{\mathbf{k}\sigma n}$, with n the band index and $\sigma = 1, 2$ representing the two transverse polarization modes of the radiation field. The magnitude of the dipolar moment is given by d_{21}, and its direction by the unitary vector $\mathbf{u_d}$. The quantization volume is represented by the constant v. In the frame of the dipolar approximation, the system interaction operator L takes the form $i\sigma_{12}$. Finally, the Hamiltonian of a two level system in contact with an electromagnetic field can be further simplified by applying the unitary transformation $U_t = e^{i[\sum_\lambda \omega_S a_\lambda^\dagger a_\lambda t + \frac{\omega_S}{2}(\sigma_{22}-\sigma_{11})t]}$ to such Hamiltonian, so that now,

$$\tilde{H}_{tot} = \sum_\lambda \Delta_\lambda a_\lambda^\dagger a_\lambda + \sum_\lambda g_\lambda(a_\lambda^\dagger L + L^\dagger a_\lambda), \tag{11.6}$$

(hereafter referred just as H_{tot} for simplicity), with $\Delta_\lambda = \omega_\lambda - \omega_A$. It is easy to verify that the stochastic and master evolution equations in the interaction picture with respect to the system, presented in the last sections, are suitable for this Hamiltonian, by only redefining the correlation function and noise as:

$$\hat{\alpha}(t) = \sum_\lambda g_\lambda^2 e^{-i\Delta_\lambda t} = e^{i\omega_A t}\alpha(t), \tag{11.7}$$

where $\alpha(t)$ was defined in Chapter (2) as

$$\alpha(t) = \sum_\lambda g_\lambda^2 e^{-i\omega_\lambda t}, \tag{11.8}$$

and

$$\hat{z}_t^* = -i\sum_\lambda g_\lambda z_\lambda^* e^{i\Delta_\lambda t} = e^{-i\omega_A t} z_t. \tag{11.9}$$

Let us now introduce the correlation function which characterizes the interaction of a two level system with the modified radiation field which lies within a PC.

11.3 THE CORRELATION FUNCTION OF THE FIELD WITHIN A PBG MATERIAL FOR A TWO LEVEL DIPOLAR COUPLING

It has been shown in the preceding parts of this thesis that an important quantity in order to characterize the action of the environment over the system, appearing in all the evolution equations (both stochastic and master), is its correlation function $\alpha(t)$. In this section, we calculate the correlation function characteristic of the dipolar coupling of a two level atom to the modified radiation field within a PC.

The correlation function we propose gives a better description of the frequencies in the middle of the band and describes the short time limit behavior more accurately than previous models [42]. This is of primary importance to describe correctly the non-Markovian effects in the dynamical equations of the quantum open system, not only in the long time scale, but also in short time limit. In order to calculate $\alpha(t)$, the sum appearing in equation (11.8) has to be performed, where $\lambda = \{\mathbf{k}\sigma n\}$ and the functions g_λ are those defined in (11.5), characteristic of a dipolar coupling. As we have already noted in the introduction, the presence of a periodic dielectric structure causes the appearance of optical bands, which are themselves periodic structures in the reciprocal lattice. In fact, the index n which now appears in the sum (11.8) denotes each band. Nevertheless, this index will be here dropped, since we consider the dynamics of the two level system with rotating frequency nearby (or inside) a single band. To describe in particular the dynamics near the edge of the band, an effective mass approximation to the full dispersion relation, based on its expansion in the vicinity of the band edge, is often considered (see for instance [42, 116, 117, 118]). Within this approximation, the dispersion relation becomes $\omega(\mathbf{k}) = \omega_c + A(\mathbf{k} - \mathbf{k}')^2$, where $\mathbf{k}'$ is the origin of the first Brillouin zone of the crystal (which is the unitary cell in $\mathbf{k}$ space [106]) about which we perform the expansion in each direction, ω_c is the frequency of the band edge, and A is a constant that depends on the specific photonic crystal considered. Although it is valid for the description of several important physical phenomena occurring in PBG materials [13, 112, 113, 114], this model of dispersion relation presents an important drawback: it becomes inaccurate for a good description of the short time dynamics. According to [42] it shows the following form,

$$\alpha(\tau) \cong \beta^{1/2}\frac{e^{i[\pi/4-\omega_c\tau]}}{\tau^{3/2}}, \tag{11.10}$$

where the constant β is determined by the integration in $\mathbf{k}$. The singularity at the origin of the last expression is non-physical. The reason is that there is no quantity z_t, which represents the fluctuations of the EM field in the stochastic model, such that its correlation function (i.e. the average value $\mathcal{M}[z_t z_\tau^*] = \alpha(t-\tau)$) is singular at the origin. There are several ways to derive dispersion relations, most of them analogous to those developed for obtaining the band structure for electrons in solids. In fact there exists a strong analogy between energy bands in solids and dispersion relations of the EM field in PBG materials [46]. In this work, we propose a model of dispersion relation (of tight-binding type) that contains all the essential features of the EM field in a photonic band gap material,

$$\omega(\mathbf{k}) = A + \frac{B}{3}\big(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\big). \tag{11.11}$$

Due to its periodic character, this dispersion relation will not show the cutoff frequency problem responsible for the appearance of the singularity at the origin in (11.10), and for short frequencies it permits the recovering of the former dispersion relations by performing the corresponding expansion in $\mathbf{k}'s$ near the band edge. In addition, the dispersion relations that has been obtained both experimentally [120] and theoretically [118, 121], are periodic functions, and not parabolic functions. The model (11.11) of dispersion relation is rather simple, and corresponds to a cubic lattice. If very precise quantities had to be computed, or if we had a photonic crystal with some other structure, then it would be mandatory to use some different or more accurate dispersion relation. However, this would neither change the methodology to derive the correlation function presented throughout this section, nor the way to compute the corresponding Gaussian noise z_t.

Figure (11.1) shows, for the direction k_x in the first Brillouin zone (1BZ), that the constants A and B, which are characteristic of material, fix the limits of the band between $\omega_c = A - B$ and $\omega_c' = A + B$. Here, we have also considered a cubic lattice with lattice constant a. Notice that in the limit of $k_i \to k_{0i}$, where $i = x, y, z$ and $k_{0i} = \pi/a$, the dispersion relation (11.11) becomes the parabolic dispersion relation above described.

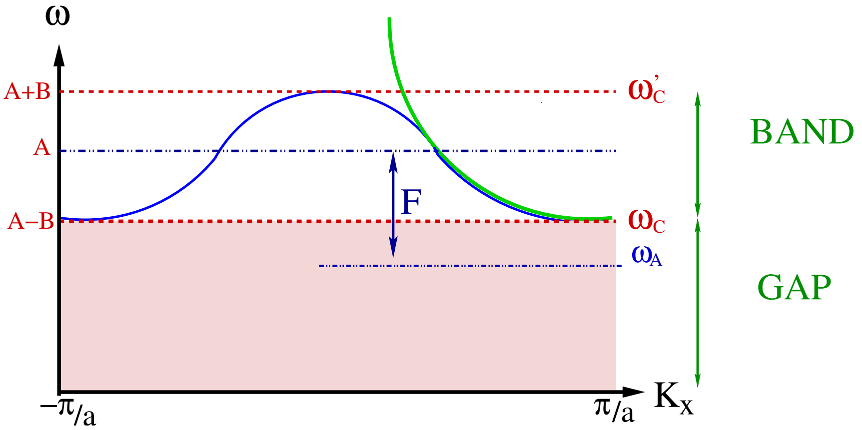

Fig. 11.1 The figure displays the band structure of the problem along one of the three directions (in particular the direction k_x) of the first Brillouin zone of the crystal. The periodic dispersion relation proposed in this work is displayed in black solid line, and the parabolic dispersion model of S.John and T. Quang. [116] in grey solid line. Notice the coincidence of both models in the limit of $k_x \to \pi/a$ (where $k_x' = \pi/a$ is the limit of the First Brillouin zone in this direction).

If we consider the continuum limit in the sum (11.8) which is performed over the $1BZ$ of the crystal, we have

$$\alpha(\tau) = \gamma(\frac{a}{2\pi})^3 \sum_\sigma \int_{1BZ} d\mathbf{k} \frac{|\hat{e}_{\mathbf{k},\sigma} \cdot \hat{u}_d|^2}{\omega(\mathbf{k})} e^{-i\omega(\mathbf{k})\tau}, \tag{11.12}$$

where $\gamma = \omega_A^2 d_{21}/2\epsilon_0$ and ϵ_0 is the free space permitivity. We now suppose that the function $|\hat{e}_{\mathbf{k},\sigma} \cdot \hat{u}_d|^2/\omega(\mathbf{k})$ changes very smoothly with $\mathbf{k}$ in the $1BZ$, and can be considered a constant factor in comparison with the rapidly oscillating exponential term. It is important to stress that although this approximation becomes more accurate in the long time limit, it is not the stationary phase approximation. In the integral (11.12), the reason why the prefactor $|\hat{e}_{\mathbf{k},\sigma} \cdot \hat{u}_d|^2/\omega(\mathbf{k})$ can be considered constant is that it changes very slowly with the wave vector $\mathbf{k}$, and this occurs no matter how large is τ in the phase $i\omega(\mathbf{k})\tau$. This fact makes the approximation valid even at short times, as can be easily verified numerically by computing the integral (11.12) both considering the prefactor in the integral or as a constant. Once we have done these simplifications, we are ready to substitute the periodic dispersion relation here proposed in the equation (11.12). Let us however, distinguish between two cases: a three dimensional band structure (as the one described with (11.11)) and a one dimensional structure in the direction denoted by k, so that now the dispersion relation becomes simply $\omega(k) = A + B\cos(ka)$.

11.3.1 Three dimensional correlation function.

For a three dimensional band structure with the periodic dispersion relation dispersion relation (11.11), the correlation function can be obtained from the equation (11.12), once it has been assumed that the function $|\hat{e}_{k,\sigma} \cdot \hat{u}_d|^2/\omega(\mathbf{k})$ is a slowly varying function in the $1BZ$. The resulting integral is analytical, and gives rise to the following result:

$$\begin{aligned}\alpha_{3D}(\tau) &\cong \gamma \sum_{\sigma} \frac{|\hat{e}_{\mathbf{k_0},\sigma} \cdot \hat{u}_d|^2}{\omega(\mathbf{k_0})} e^{-iA\tau} J_0^3(\frac{B\tau}{3}) \\ &\cong g_{3D}^2 e^{-iA\tau} J_0^3(\frac{B\tau}{3}), \qquad (11.13)\end{aligned}$$

where $\mathbf{k_0}$ is again a fixed point located in the three dimensional interval $[0, \mathbf{k}']$. The function (11.13) is displayed in Fig. (11.2) for various values of A (or, equivalently, for various values of F, since $A = \omega_S - F$, and we take $\omega_S = 1.$ as explained in the next section).

In order to compare with previously established results, we perform the long time limit expansion of the last equation,

$$\begin{aligned}\alpha(\tau \gg 1)_A &\sim g_{3D}^2 e^{-iA\tau} (\frac{6}{B\tau})^{3/2} [\frac{e^{i(\frac{B\tau}{3}+\frac{\pi}{4})} + e^{-i(\frac{B\tau}{3}+\frac{\pi}{4})}}{2}]^3 \qquad (11.14) \\ &\approx \frac{g^2}{8} e^{-i\omega_c\tau} (\frac{6}{B\tau})^{3/2} e^{-i\frac{3\pi}{4}},\end{aligned}$$

and comparing with (11.10), we establish the following relation between constants:

$$\beta^{1/2} = \frac{g_{3D}^2}{8} (\frac{6}{B})^{3/2}, \qquad (11.15)$$

where also $e^{i\pi/4} \equiv e^{-i3\pi/4} \equiv 1/(i)^{3/2}$. Equation (11.13) is therefore not only valid in the long time limit as previous proposals, but gives more accurate description of the short times.

11.3.2 One dimensional band correlation function.

Let us suppose now that we are dealing with a one dimensional band. This band can be created in a photonic crystal in which the periodicity of the refraction index occurs only along one direction, for instance by alternating layers of high and low refraction index . For this one dimensional band, equation (11.12) becomes,

$$\alpha(\tau)_{1D} \cong \gamma(\frac{a}{2\pi}) \sum_{\sigma} \frac{|\hat{e}_{k_0}\sigma(R) \cdot \hat{u}_d|^2}{\omega(k_0)} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk e^{-i(A+B\cos(ka))\tau}. \qquad (11.16)$$

After the integration, the one dimensional correlation function is given by

$$\alpha(\tau)_{1D} \cong \gamma \sum_{\sigma} \frac{|\hat{e}_{k_0}\sigma(R) \cdot \hat{u}_d|^2}{\omega(k_0)} e^{-iA\tau} J_0(B\tau), \qquad (11.17)$$

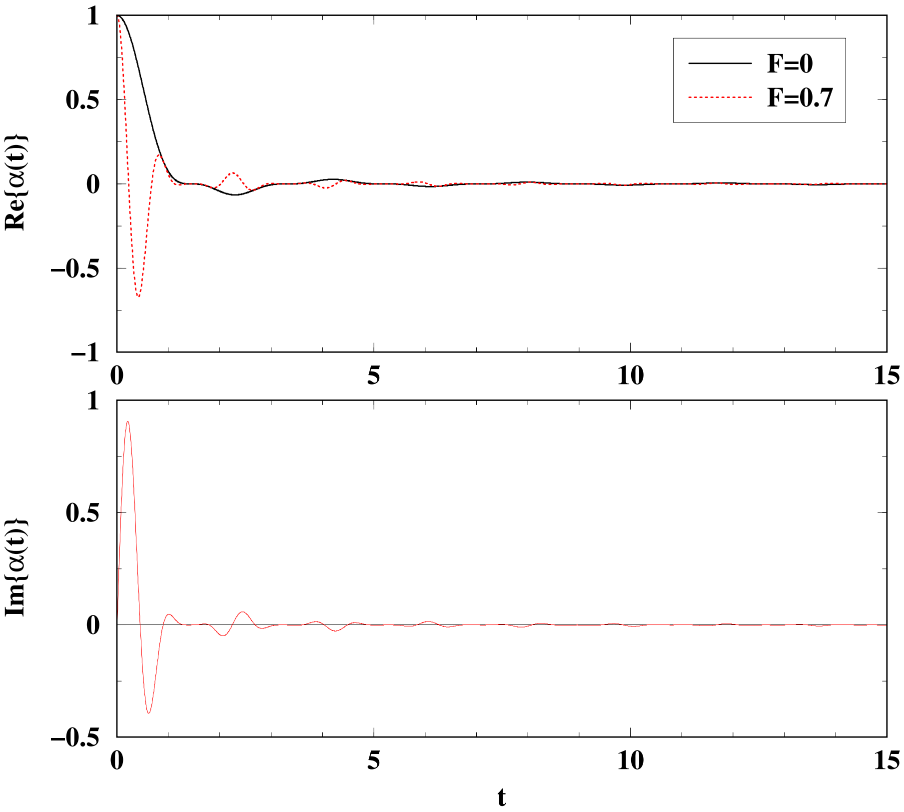

Fig. 11.2 The figure displays the real and imaginary part of the correlation function (11.13) for different values of $A = \omega_S - F$. Particularly, for $A = 1$, which corresponds to the atomic frequency within the band $F = 0$, and $A = 0.3$, which corresponds to the atomic frequency within the gap $F = 0.7$. It can be observed in both figures the long time decaying τ_c of the correlation function, which produces a highly non-Markovian interaction.

where J_0 is the zero order Bessel function. Considering the long time limit of (11.17), we have

$$\begin{aligned}\alpha(\tau \gg 1)_{1D} &\sim g_{1D}^2 e^{-i\omega_c\tau}(\frac{2}{B\tau})^{1/2}(\frac{e^{-i\frac{\pi}{4}} + e^{-i2B\tau}e^{i\frac{\pi}{4}}}{2}) \\ &\approx g_{1D}^2 e^{-i\omega_c\tau}(\frac{1}{2B\tau})^{1/2}e^{-i\frac{\pi}{4}},\end{aligned} \quad (11.18)$$

where we have neglected the more rapidly oscillating terms in $2B$.

11.4 TYPICAL VALUES OF THE MAGNITUDES INVOLVED IN THE PROBLEM

Before starting with the discussion, let us give first an idea of the values of the different physical magnitudes involved in the problem. As we have already sketched in the Introduction, PCs typically consist of a low-dielectric-constant network, inserted in a high-dielectric-constant backbone in an specific structure. There are several works containing band structure numerical calculations in which numerous structures exhibiting band-gap are proposed (see for instance [122, 46] for a good review). These studies are often compared to the experimental data, which is mainly based on the analysis of the reflection and transmission spectra of the material. A large variety of these structures give rise to a complete 3D band gap. Some examples are the inverse diamond structure formed by overlapping air spheres in a dielectric material [123], the woodpile structure (a variation of the diamond structure) [124], SiO_2 spheres in a InP backbone [125], or spiral shaped rods arranged in simple cubic (SC), face-centered cubic (FCC) on any body centered cubic (BCC) lattices [126]. For an extended review of the current state of photonic band structure theory, both experiments and applications, see [122, 46]. Of special interest for optical applications are the PCs with the photonic gap in the IR and visible regimes. One of the most recently developed PC with an optical PBG, consists in silica spheres, with diameters between 600 and 1000 nm, periodically inserted in bulk silicon [120]. The size and disposition of the spheres gives rise to the formation of a 5% complete 3D PBG centered near 1.5 μm, which has been experimentally observed. We will use in our study appropriate values for the parameters that characterize the photonic crystal in the optical regime ($\omega_A \approx 10^{15}$ Hz, $d_{21} \approx 10^{-29}$Cm, $a \approx 10^{-6}$m, $\omega_c \approx 2.33 \cdot 10^{15}$Hz and $B = 0.5 \cdot 10^{15}$Hz.). With these parameters, $g_{1D} \approx g_{3D} \approx 0.1 \cdot 10^{15}$Hz. As we have mentioned above, the coupling constant is such that H_I is equivalent in magnitude to gH_0. But H_0 has approximately the magnitude of the atomic frequency, ω_A, and this is how, from the values of $g_{1D,3D}$, we can deduce that $g \approx 0.1$. For simplicity, we will consider ω_A as the unit frequency of the problem.

12

Quantum mean values and fluctuations

We describe in this chapter the evolution of single quantum mean values of a two level atom within a photonic crystal. The chapter is divided in two sections, each of which concerns the study of the spontaneous emission and the emission of the atom when in addition to the interaction with the electromagnetic field it is driven by a laser. The main points treated can be summarized as follows:

- We provide a dynamical description of the problem in terms of the stochastic Scrödinger equation formalism, within the second order perturbation theory. As already mentioned, in order to do that it is necessary to have a good description of the environmental fluctuations, which are represented by the noise in the stochastic equations. To this end, the use of the non-singular correlation function defined in the former chapter is very convenient. We show how some of the physical effects already described in literature [42], are correctly reproduced with the stochastic formalism and the new correlation function we propose. Those effects, as well as the sections where they are treated are the following,
    - In Section (12.2) we examine the atomic residual long time limit population and photon-atom bound state, when the atomic rotating frequency is placed within the gap region of the photonic DOS. We also show the non-exponential decay of the upper level population when the atomic rotating frequency is within the band.
    - In Section (12.3), the effects of a strong laser field in this system are studied. Particularly, we show the conditions under which population inversion appears in the long time limit.
- We compare the second order perturbative approximation in the weak coupling parameter with the solution given by the equation obtained with the expansion approximation discussed in Section (2.4.1). The expansion equation seems to describe with more accuracy the system dynamics when the rotating frequency is in the band edge. At least, it seems to reproduce a residual long time limit population of the excited level, an effect that was previously described by S. John with an exact model. This is not observed in the second order perturbative approximation. The reason is that in the band edge region such approximation is not appropriate, since the photonic DOS varies very rapidly from a non-zero to a zero value.

12.1 GENERAL DYNAMICAL EQUATIONS

We present here briefly the dynamical equations we are going to use in this chapter to describe the problem. Since we consider $T = 0$, it is convenient to use a linear stochastic equation (12.1), which in interaction image with respect to the system is

$$\frac{d}{dt}|\psi_t(z^*)\rangle = gV_tLz_t^*|\psi_t(z^*)\rangle - g^2V_tL^\dagger \int_0^t d\tau\alpha(t-\tau)V_\tau L|\psi_t(z^*)\rangle, \tag{12.1}$$

where $V_tL = \exp{(iH_At)}L\exp{(-iH_At)}$. As usual, the reduced density matrix can be computed from $|\psi_t(z^*)\rangle$ as

$$\rho_s(t) = \frac{\mathcal{M}[|\psi_t(z^*)\rangle\langle\psi_t(z)|]}{\mathcal{M}[\langle\psi_t(z)|\psi_t(z^*)\rangle]}. \tag{12.2}$$

We also use the two models of master equation described in Section (5.1.1.1), namely the non-convoluted master equation (5.66), which is derived by performing analytically the ensemble over the projector $\mathcal{P}_t = |\psi_t(z^*)\rangle\langle\psi_t(z)|$,

$$\begin{aligned}\frac{d\rho_t}{dt} &= g^2L(t)\rho_t\int_0^t d\tau\alpha^*(t-\tau)L^\dagger(\tau) + g^2\int_0^t d\tau\alpha(t-\tau)L(\tau)\rho_tL^\dagger(t)\\ &- g^2L^\dagger(t)\int_0^t d\tau\alpha(t-\tau)L(\tau)\rho_t - g^2\rho_t\int_0^t d\tau\alpha^*(t-\tau)L^\dagger(\tau)L(t),\end{aligned} \tag{12.3}$$

and a convoluted master equation (5.71), which is identical to the last one by only replacing ρ_t by ρ_τ in the terms,

$$\begin{aligned}\frac{d\rho_t}{dt} &= g^2L(t)\int_0^t d\tau\alpha^*(t-\tau)\rho_\tau L^\dagger(\tau) + g^2\int_0^t d\tau\alpha(t-\tau)L(\tau)\rho_\tau L^\dagger(t)\\ &- g^2L^\dagger(t)\int_0^t d\tau\alpha(t-\tau)L(\tau)\rho_\tau - g^2\int_0^t d\tau\rho_\tau\alpha^*(t-\tau)L^\dagger(\tau)L(t).\end{aligned} \tag{12.4}$$

As noted in Section (5.1.1.1), both master equations (convoluted and non-convoluted) are equivalent up to second order in g. As we will show in Section (12.2.2), a remarkable difference in the result derived from a convoluted and a non-convoluted equation will therefore indicate a failure in the second order perturbative approximation.

12.2 TWO LEVEL ATOM SPONTANEOUS EMISSION

We have just established in Chapter (11) the Hamiltonian of the two level system within the modified radiation of a PBG material, and also the typical magnitudes involved in the problem. Let us now start with the study of the dynamics of the two level system for the three dimensional correlation function (11.13).

We are concerned first in reproducing, using the correlation (11.13), the non-zero steady state population effect shown in [42] for an atom with resonant frequency inside the gap. For the atomic frequency inside the band, we will also point out some restrictions to the validity of the second order perturbative approximation for this model. The second and main goal of this section will be to show that, according to equation (12.2), the master equation results can also be obtained with an ensemble average of the solutions of the stochastic linear equations described above. Finally, we will study some aspects and properties of individual stochastic trajectories. For the system interaction operator $L = i\sigma_{12}$, the non-convoluted stochastic equation in interaction image (12.1) reads as follows,

$$\begin{aligned} \frac{d|\psi_1(t)\rangle}{dt} &= g z_t^* |\psi_2(t)\rangle \\ \frac{d|\psi_2(t)\rangle}{dt} &= -g^2 \int_0^t d\tau \hat{\alpha}(t-\tau)|\psi_2(t)\rangle, \end{aligned} \tag{12.5}$$

with $\hat{\alpha}(t-\tau)$ and $\hat{z}_t^*$ defined in (11.7) and (11.9) respectively, and $|\psi(t)\rangle = \{|\psi_1(t)\rangle, |\psi_2(t)\rangle\}$ representing the two spinorial components of the two level system stochastic wave function. The non-convoluted master equation (12.3) becomes, for each term of the density matrix, the following,

$$\begin{aligned} \frac{d\rho_{11}(t)}{dt} &= 2g^2 \int_0^t d\tau \Re\{\hat{\alpha}(t-\tau)\}\rho_{22}(t) \\ \frac{d\rho_{12}(t)}{dt} &= -g^2 \int_0^t d\tau \hat{\alpha}^*(t-\tau)\rho_{12}(t) \\ \frac{d\rho_{22}(t)}{dt} &= -2g^2 \int_0^t d\tau \Re\{\hat{\alpha}^*(t-\tau)\}\rho_{22}(t). \end{aligned} \tag{12.6}$$

As we have already mentioned, up to the second order approximation, the master equation (12.6) is equivalent to the convoluted master equation, in which the only difference is that each of the components ρ_{ij} that appear in the integral terms depend on τ, i.e. are part of the integrands. In addition to that, the convoluted equation is equal to the one calculated in [42] by M. Florescu and S. John for the same model. A difference in the result of the convoluted and the non-convoluted equation must be related with the fact that the second order perturbative approximation is no longer valid. As will be shown in the next section, the range of validity of such approximation depends not only on the coupling constant g, but also on the correlation time of $\alpha(t)$. In our model, such correlation time is approximately given by $1/B^{3/2}$, where $2B$ is the band width.
Let us now introduce the parameter that characterizes the situation of the atomic frequency with respect to the band. According to its definition (11.7) in terms of $\alpha(t-\tau)$, the function $\hat{\alpha}(t-\tau)$ appearing in the evolution equations depends on $F = \omega_A - A$ (see Fig. (11.1)), which is the detuning between the atomic rotating frequency ω_S and the frequency of the center of the band A. Indeed, when $-B < F < B$, the atomic rotating frequency is placed within the band, whereas it will lay within the gap when $|F| > B$. Let us consider, as indicated, the evolution of $\rho_{22}(t)$ in these two cases. Since the photon density of states is zero, no propagating modes are allowed. This means that there are no extended states expressible in Bloch form. Instead, the wave vector is pure imaginary, and the modes decay exponentially in space forming a localized state. When the rotating frequency ω_A of an excited two level atom is placed inside the gap, and the atom drops to the ground state through a single-photon spontaneous emission, the emitted photon will be in a localized state corresponding to one of these purely imaginary wave vectors. The result of this localization is a strong coupling between the electronic degrees of freedom of the atom and the electromagnetic modes of the localized field, namely, the photon-atom bound state first predicted by John and Wang [117, 118]. On the other hand, in the region near the band border, the photon density of states decays to zero, and therefore the group velocity $d\rho(\omega)/d\omega$ vanishes. In consequence, when the atomic frequency is placed nearby the band edge, ω_c, the atom will be coupled to photons with vanishing group velocity. In this case, the self-dressing of the atom with its own radiation is strong enough to produce a splitting of the atomic level into a doublet. One member of the doublet is pulled inside the band, where it experiments spontaneous emission, whereas the other remains in the gap, retaining the photon-atom bound state. The interference between the doublets causes the oscillatory behavior described in [42] and observed in the inset of fig. (12.1).

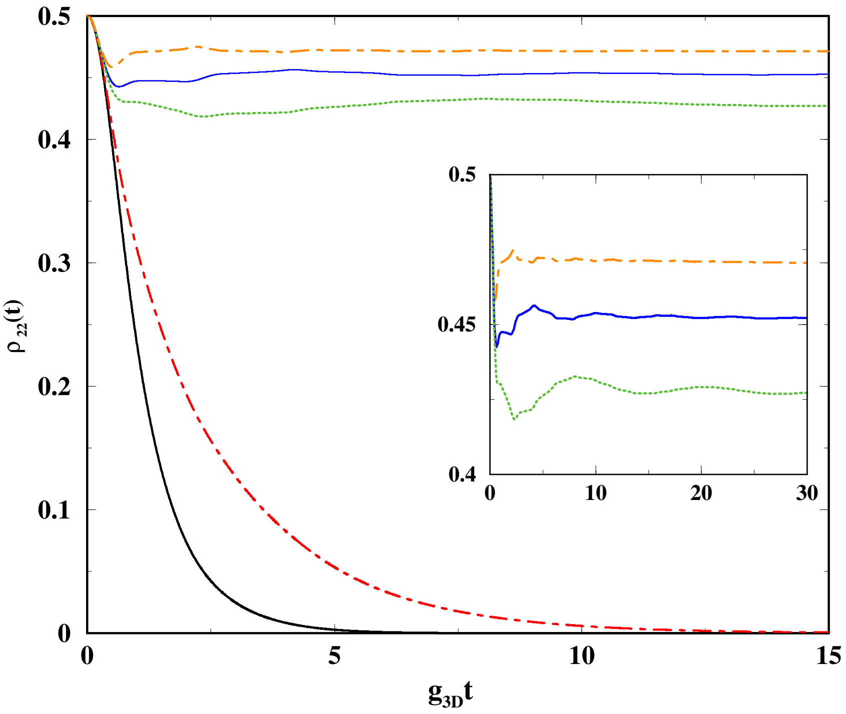

Fig. 12.1 The atomic population of the excited state, $\rho_{22}(t)$, as a function of the scaled time $g_{3D}t$, for various values of $F = \omega_A - A$. In black, the solutions corresponding to ω_A inside the band (solid line for $F = 0$ and dot-dashed line for $|F| = 0.3$) present a vanishing excited population. In change, when ω_A lies inside the gap, a non-zero steady state excitation amplitude can be observed (in grey) for different values of the detuning (dotted line for $|F| = 0.55$, dot-dashed line for $|F| = 0.6$ and solid line for $|F| = 0.7$). These values of the atomic population inside the gap are displayed in more detail in the inset of the figure. The oscillations observed are due to the energy exchange between the atomic splitted levels, produced by the atomic self-dressing.

Another effect of the photon-atom bound state, also shown in fig. (12.1), is that the atomic excited level population is non zero in the steady state. Indeed, because the emitted photon localizes within a certain region nearby the atom, it has a certain probability to be reabsorbed by the atom, producing in consequence its re-excitation. According to [46, 118], the localization region nearby the atom is defined by a certain localization length ζ_{loc}, which depends on the situation of the atomic frequency ω_S with respect to the band-edge ω_c as $\zeta_{loc} \propto c/\sqrt{\omega_c|\omega_c - \omega_A|}$. This relation shows that ζ_{loc} is larger when approaching to the edge ω_c, which means that the photon probability becomes more extendedly distributed in the space. In this situation, it becomes less probable for the photon to be reabsorbed by the atom, and the mechanism of re-excitation of the atom becomes less efficient than in the region which is deeper inside the gap. A consequence of this effect is shown in fig. (12.1), which displays a smaller long time limit population as ω_S approaches to the ω_c. Attending to the other possibility, when the atomic frequency is placed inside the band, the atomic excited population decreases up to a zero value in steady state. This result, displayed in fig. (12.1), is expected to be correct in all regions of the band except in the border, where according to more accurate descriptions [113, 117], a residual non-zero steady state population should be expected. This inaccuracy is due to the fact that the low order perturbative approximation results particularly unsuitable in the border area, where the photonic density of states rapidly increases. Some restrictions and validity conditions of the second order perturbative approximation will be established in Section (12.2.2.1).

12.2.1 Time evolution of populations obtained from the stochastic Schrödinger equation

In the last section, we have established the validity of a non-singular correlation function, such as (11.13), to describe the dynamics of a two level atom with resonance frequency near or inside a photonic band gap. We now study the solutions of the corresponding stochastic equation (12.5), both statistically (comparing the ensemble averaged solutions with that of the master equation (12.6)), and in terms of single trajectories. We will focus on the result obtained with the spinor $|\psi_1(t)\rangle$, which according to the stochastic equation (12.5) includes all the dependence over the stochastic variable. In particular, in fig. (12.2) is shown the evolution of the element $\rho_{11}(t)$ obtained from the ensemble average $\mathcal{M}[P_1 1] = \mathcal{M}[|\psi_1(t)\rangle\langle\psi_1(t)|]$ over a different number of trajectories, κ. Indeed, for the two cases studied (atom frequency in the gap, with $|F| = 0.7$, or in the band, with $F = 0$), and provided that κ is large enough, a convergence to the master equation solution is observed. In fig. (12.2) it is also observed that when $F = 0$ the statistics are considerably better than with $|F| = 0.7$, and only a small number of trajectories is needed to recover the average value. A possible explanation is found by studying the behavior of a single trajectory in each case. As shown in fig. (12.3) (top), stochastic trajectories inside the band reduce to a certain state in which the stochastic driving term no longer affects. This corresponds to a situation in which the coherences of the density matrix (see fig. (12.3) below) have been destroyed by the interaction. Naturally, the ensemble average of such solutions will be very efficient, as the fluctuation disappears at relatively short times. In contrast, in the single trajectory corresponding to $|F| = 0.7$, i.e. atomic frequency inside the gap, the fluctuation term remains important during the whole evolution. This corresponds to the special situation created inside the gap, in which the atomic coherences are not destroyed, as they would if the atom were in the band, or even in the vacuum. The relation between the coherences of $\rho(t)$ and the stochastic forcing can be more clearly seen in equation (5.68), where the noise terms are accompanied by $L(t)$ and $L^\dagger(t)$ (let us remind here that $L = i\sigma_{12}$).

12.2.2 Validity of the perturbative approximation

12.2.2.1 *Study of the positivity* As noted in Chap (2), a physical condition to be satisfied by proper solutions is that the transition probability $P_{1\to 2}(t)$, from the lower state $|1\rangle$ to the upper state $|2\rangle$, is positive and smaller than one ($0 < P_{1\to 2} < 1$). Such probability is given by the averaged projector $\mathcal{M}[|\psi_2(t)\rangle\langle\psi_2(t)|]$,

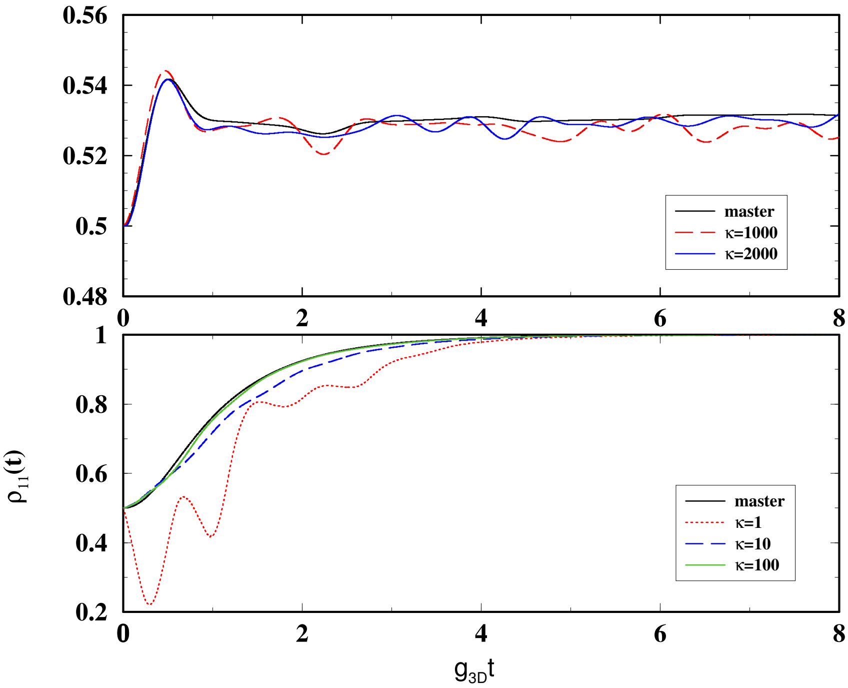

Fig. 12.2 Ensemble averaged values of the stochastic equation $\mathcal{M}[|\psi_1(t)\rangle\langle\psi_1(t)|]$ for different number of trajectories, compared with the result of the (non-convoluted) master equation. Each time step represent around ten atomic transitions. In the upper figure, corresponding to $|F| = 0.7$ (atomic bare state frequency inside the gap), the average corresponding to $\kappa = 2000$ trajectories has a relative error less than ≈ 0.008 in the scale. In the lower graph, which corresponds to a situation in which ω_A is in the band, a relative error approximately inferior to 0.02 is reached with only $\kappa = 100$. Clearly, this situation presents a considerable improvement in the statistics in comparison with the case in which ω_S is within the gap.

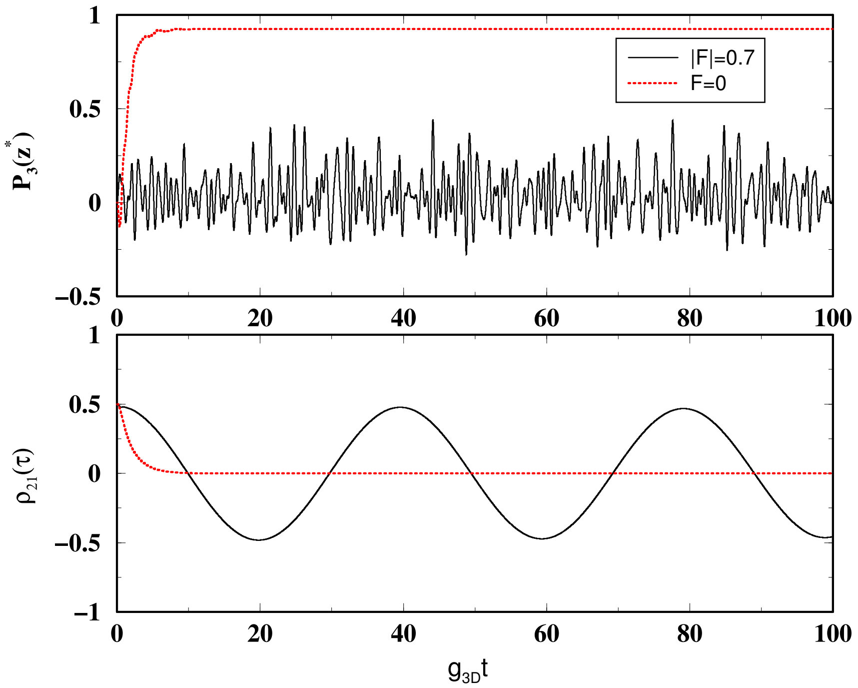

Fig. 12.3 The upper figure represents the time evolution of the stochastic projector, $P_3 = P_{22} - P_{11}$ corresponding to a single trajectory. The two curves appearing in such figure correspond to $|F| = 0.7$ and $F = 0$ respectively. The figure below represents the density matrix coherence ρ_{21} in the same time scale. It displays the same two cases as the figure above. Observing both figures, the vanishing of the stochastic forcing is found to be related to the suppression of coherences, a process that apparently only occurs within the band. The absence of spontaneous emission which occurs in the gap might be a possible explanation of the survival of the density matrix coherences and, in consequence, of the stochastic driving.

or equally, by the element $\rho_{22}(t)$ of the density matrix. As a secondary effect, unphysical solutions with $P_{1\to 2}(t) > 1$, correspond to non-positive values for the density matrix, i.e. with $det\{\rho_t\} < 0$. However, let us note here that none of such problems appear when the density matrix is calculated through averaged solutions of stochastic equation. The reason comes precisely from the definition (12.2), in which this matrix is calculated through an averaged sum of projectors and therefore preserves positivity. In consequence, we will base our test of validity of the second order perturbative approximation in the master equation solutions. The calculus is identical to that performed in Section (2.4.4), where it was settled that the limit condition in which the convoluted master equation (12.4) for $\rho_{22}(t)$,

$$\frac{d\rho_{22}(t)}{dt} = -2g^2 \int_0^t d\tau \Re\{\hat{\alpha}(t-\tau)\}\rho_{22}(\tau) + \mathcal{O}(g^3), \tag{12.7}$$

is positive. The solution of the former equation is given by

$$P_{1\to 2}(t) = \rho_{22}(t) = \rho_{22}(0)\left[1 - 2g^2 \int_0^t dl \int_0^l d\tau \Re[\hat{\alpha}(l-\tau)\right] + \mathcal{O}(g^4). \tag{12.8}$$

Having non-negative transition probabilities implies that the integral term on the right hand side of the last equation is positive and less or equal to one. Considering the more restrictive condition in which $\rho_{22}(0) = 1$, the maximum time t_m in which such condition is fulfilled, is defined as follows,

$$\frac{1}{g^2} = 2\int_0^{t_m} dl \int_0^l d\tau \Re[\hat{\alpha}(l-\tau)]. \tag{12.9}$$

On the other hand, the non-convoluted version or the equation (12.3) has the following second order solution:

$$P_{1\to 2} = \rho_{22}(t) = \rho_{22}(0)e^{-2g^2 \int_0^t dl \int_0^l d\tau \Re\hat{\alpha}(l-\tau)}. \tag{12.10}$$

The double integral in the last expression is performed over the *real part* of the correlation function, and therefore $P_{1\to 2}$ is always a positive quantity. On the other hand, for the correlation functions (11.13) and (11.17), the double integral itself is positive, and so $P_{1\to 2}$ is also less than one. The fact that convoluted master equation solutions do not preserve positivity, as follows from (12.8), whereas stochastic and non-convoluted master solutions preserve it, as it is shown in (12.10), reflects by itself the failure of the second order approximation. Only by considering that the second order approximation is no longer valid, can we explain the difference between the result of the convoluted master equation and the stochastic and non-convoluted master equations. Equation (12.9) shows clearly that the validity of the second order perturbative approximation depends on the magnitude of g. However, as we have mentioned above, another parameter to consider is the correlation time τ_c of $\hat{\alpha}(t-\tau)$. For a fixed value of g, we changed the band width (that goes inversely with the correlation time), verifying that the negative values of the density matrix of the convoluted master equation, (or analogously, the values in which $P_{1\to 2}(t) > 1$ or $P_{1\to 2}(t) < 0$) tend to disappear as τ_c decreases. The smaller the correlation time, the longer is the time limit t_m up to which the second order perturbation theory remains valid. Finally, we also observed that the violation of positivity (or the violation of the condition over $P_{1\to 2}$) only occurs when the atom frequency lies inside the band, an effect that can be easily explained as follows. Because the photon density of states (DOS) increases very rapidly in the band, becoming larger than in the vacuum, such region results especially problematic for a perturbative approach. This can be seen in fig. (12.4), where for the mid-band values ($F = 0$) the DOS becomes so large that the perturbative approach presents some problems, as reflected by the difference between the curves corresponding to two different equations equivalent in this order. Notice however, that there is a connection between the band width and the shape of the photonic DOS. In particular, the larger the band width B, the smaller is the variation of the photonic DOS in comparison to the spontaneous emission rate. This corresponds to a situation where the Markovian approximation becomes more suitable, which makes a perturbative approximation more suitable.

We can have a more clear insight of these effects (dependence of the validity of perturbative theory on τ_c and, in the case of PBG, dependence on position of the atom frequency), by calculating analytically the condition (12.9) for the simplest correlation function (11.17), which corresponds to the one dimensional band-gap structure. To this purpose, we also considered the Redfield limit of (12.7), which is based on the fact that the integral limit of the coefficient can be extended to infinity, provided that the relaxation time of the bath is still small compared to that of the system. Using the value of the Laplace transform of $J_0(x)$

$$\int_0^\infty dx J_0(bx)e^{-px} = \frac{1}{\sqrt{p^2+b^2}}, \tag{12.11}$$

valid for $\Re\{p\} > 0$, we arrive to the following expression for the maximum time t_m in which solutions preserve positivity,

$$\frac{1}{g^2} = \Re\left\{\frac{2t_m}{\sqrt{B^2-F^2}}\right\}, \tag{12.12}$$

for values of F within the band, i.e. $-B < F < B$. Expression (12.12) shows that when B is bigger (so τ_c smaller), the maximum time of validity of the perturbative hypothesis t_m is allowed to be larger.

For rotating frequencies inside the gap, $|F| > B$, the expression $\sqrt{B^2-F^2}$ is pure imaginary, and the perturbative solution (12.8) is always valid, without a restriction over the perturbative parameter such as (12.12).

12.2.2.2 Comparison of the expansion equation and the perturbative equation

The above discussion about the perturbative approximation can be useful to detect some situations in which such approximation is not valid. We present in this section a comparison of the second order perturbative equation with an equation derived in Section (2.4.1). It is important to note that this equation is not exact, as it is derived by assuming as an ansatz a particular expansion for the operator $L(\tau, t_{i+1})$. In consequence, it can not be argued that it is better than the second order perturbative equation. The only thing we can say when comparing both of them, is that the expansion equation seems to describe a residual long time limit population in the band border, as is expected from more accurate models than the perturbative one.

Let us briefly mention agein the derivation of the expansion equation derived in Section (2.4.1). In order to obtain a closed equation, the term $\langle z_i|\mathcal{U}_I(t_i,t_{i+1})L(\tau,t_{i+1})|z_{i+1}\rangle$ of the open equation of the reduced propagator (2.40) has to be manipulated. As noted above, we can assume the following expansion of the coupling operator (see Sections (2.4.1) and (9.4.2) for more details) as an ansatz,

$$L(\tau,t_{i+1}) = \sum_\alpha F_\alpha(\tau,t_i,\{a_\lambda\})S_\alpha(t_i,t_{i+1}), \tag{12.13}$$

where the set $\{S_i\}$ represent a basis of system operators, and $F_\alpha(\tau,t_i,\{a_\lambda\})$ is a certain set of operators of the total Hilbert space. For a simple mean value, $z_i = z$, $t_i = t$, $z_{i+1} = 0$, and $t_{i+1} = 0$. In addition, for $L = \sigma_{12}$, the expansion takes the simple form $L(\tau,0)|0\rangle = f(\tau,t)L(t,0)|0\rangle$, so that the term $\langle z|\mathcal{U}_I(t,0)L(\tau,0)|0\rangle = f(\tau,t)L\langle z|\mathcal{U}_I(t,0)|0\rangle$, and therefore the resulting value of the operator O is $O_e(t,\tau) = f(\tau,t)L$. From the Heisenberg motion equations, we get

$$\frac{df_e(t,\tau)}{dt} = (i\omega_S + R_e(t))\,f_e(t,\tau), \tag{12.14}$$

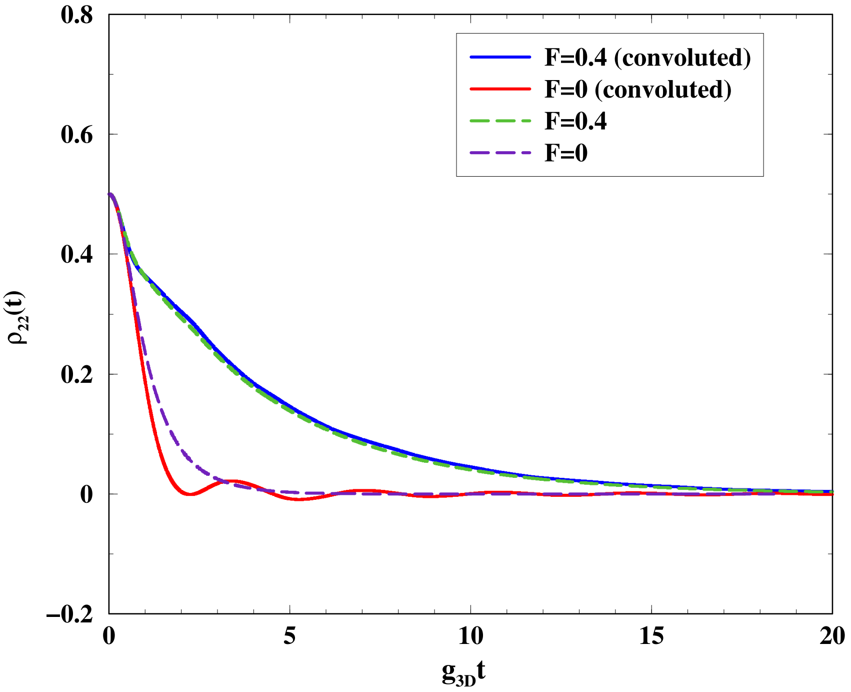

Fig. 12.4 Evolution of $\rho_{22}(t)$ for different values of $|F| < 0.5$ using the convoluted master equation (12.4), and the non-convoluted master equation (12.3). The difference between both equations becomes larger for $F = 0$, which could be explained because within that central region the the photonic DOS is so large that the perturbative approximation is no longer valid.

with $R_e(t) = \int_0^t \tau\alpha(t-\tau)f_e(t,\tau)$. The subindex e accounts for the fact that, once the last expression is replaced in equation (2.40), a closed equation is obtained for the reduced propagator that comes from the *expansion* (12.13). This equation gives rise to quantum mean values that we are interested in comparing with those obtained in the last sections and in [42, 6] with second order perturbative equations. Considering that the dissipative term of (2.40) is already of order g^2, a second order equation is obtained by only replacing $\langle z|\mathcal{U}_I(t,0)L(\tau,0)|0\rangle = f_p(\tau,t)L\langle z|\mathcal{U}_I(t,0)|0\rangle$, with

$$\frac{df_p(t,\tau)}{dt} = i\omega_S f_p(t,\tau), \tag{12.15}$$

where the subindex p accounts for the perturbative approximation. In this approximation, a zero order expansion of $L(\tau,0)$, is simply $L(\tau,0) = \exp{(iH_{tot}\tau)}L\exp{(-iH_{tot}\tau)} = V_\tau L + \mathcal{O}(g)$. In the notation of the operator O, in which $\langle z|\mathcal{U}_I(t,0)L(\tau,0)|0\rangle = O(0,z^*,t,\tau)\langle z|\mathcal{U}_I(t)|0\rangle$, the latter results can be written as $O(0,z^*,t,\tau) \equiv O(t,\tau) = f_{e,p}(t,\tau)L$, where the solution obtained with the expansion of the coupling operator, $f_e(t,\tau)$ given by (12.14), corresponds to $L = \sigma_{12}$, while the perturbative solution $f_p(t,\tau) = V_{\tau-t}L$ is valid for any coupling L. Then, for $O(0,z^*,t,\tau) \equiv O(t,\tau)$, a closed form for the equation (2.40) is

$$\begin{aligned} \frac{d}{dt}|\psi_t(z^*)\rangle &= -iH_S|\psi_t(z^*)\rangle + gLz_t^*|\psi_t(z^*)\rangle \\ &- g^2L^\dagger\int_0^t d\tau\alpha(t-\tau)O(t,\tau)L|\psi_t(z^*)\rangle. \end{aligned} \tag{12.16}$$

Once we have a closed equation for the reduced propagator, we can construct the reduced density operator of the system, $\rho_s(t) = Tr_B\{\rho_{tot}(t)\}$, as (12.2). As previously done in Chapter (5), a master equation can be computed by performing the average $\mathcal{M}[\cdots]$ analytically. For that purpose, we replace (12.16) into the equation

$$\frac{d}{dt}\rho_s(t) = M\left[\left(\frac{d}{dt}|\psi_t(z^*)\rangle\right)\langle\psi_t(z)| + |\psi_t(z^*)\rangle\left(\langle\frac{d}{dt}\psi_t(z)|\right)\right], \tag{12.17}$$

in any of the two versions, the expansion model and the perturbative. Since in any case the operator O does not depend on z, the procedure is analogous to that followed in Section (5.2.1), and gives rise to the following master equation,

$$\begin{aligned} \frac{d\rho(t)}{dt} &= i[H_S,\rho] + L\int_0^t d\tau\alpha^*(t-\tau)\rho(t)O^\dagger(t,\tau) \\ + &\int_0^t d\tau\alpha(t-\tau)O(t,\tau)\rho(t)L^\dagger - L^\dagger\int_0^t d\tau\alpha(t-\tau)O(t,\tau)\rho(t) \\ - &\int_0^t d\tau\rho(t)\alpha^*(t-\tau)O^\dagger(t,\tau)L. \end{aligned} \tag{12.18}$$

In the perturbative case, the operator $O(t,\tau)$ is given by (12.15), valid for any L, and the resulting equation is equal to (5.66) computed in Section (5.2.1). For $L = \sigma_{12}$ the operator O is given by (12.14) once the expansion (12.13) is assumed [1]. The solutions from the expansion and the perturbative model of equation (12.18) are displayed in Fig. (12.5) for the band case, where $|F| < 0.5$. Special emphasis is placed on the study of the border of the band, where the perturbative approximation is no longer valid due to the high

---

[1] We stress that the expansion (12.13) is standard for any coupling L, but the equation (12.14) is special for $L = \sigma_{12}$

values that the photonic DOS has in this region. Contrary to the perturbative model, the expansion model shows that there is population in the long time limit for frequencies within the band border, in such a way that the *effective* band border is not placed at $F = 0.5$ but deeper in the band, around $F = 0.37$ (see figure (12.7)).

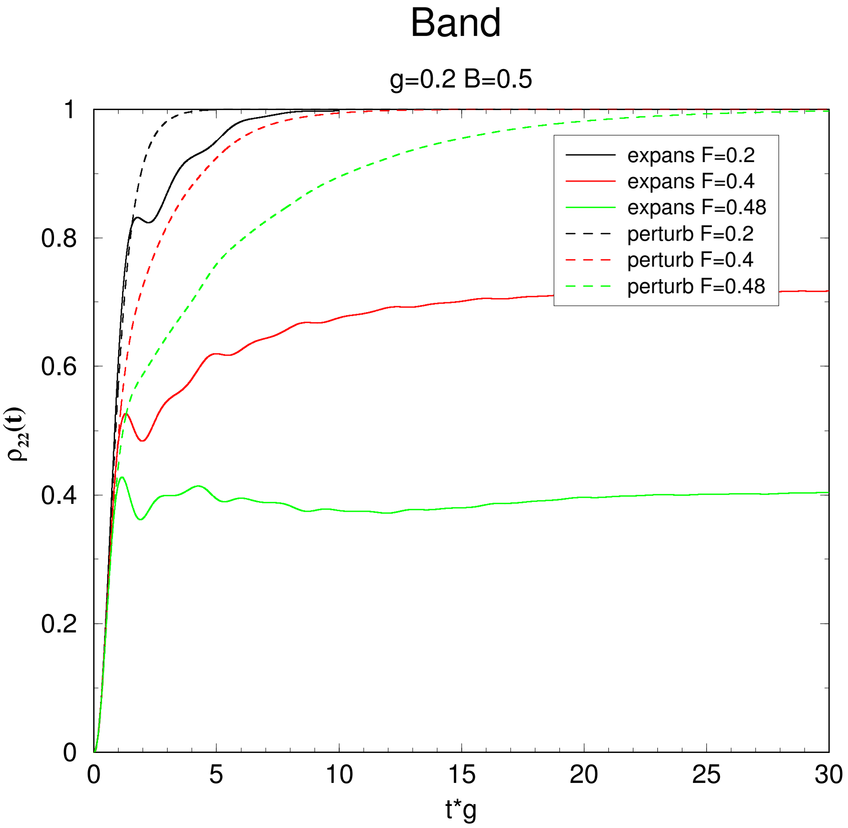

Fig. 12.5 Evolution of $\sigma_z(t)$ for $|F| < 0.5$ for the expansion and perturbative model. The difference between both models becomes specially dramatic in the border of the band, where the photonic DOS is so large that the perturbative approximation is no longer valid. Near the border of the band the asymptotic value of σ_{22} is zero whereas the expansion equation reflects already a certain residual population.

Although the photonic DOS is zero in the gap region, for frequencies placed sufficiently near the band edge the perturbative solutions differs considerably from the exact model ones. When a photon is emitted within the gap, it remains localized in a region nearby the atom and interacting with it in such a way that a so-called photon-atom bound state is formed [42]. Within that region the photon can tunnel through a certain scale in frequencies, which is larger the closer the atomic frequency is to the band edge, in such a way that there is a certain probability for the photon to be reabsorbed by the band extended modes [46]. This is how the photonic DOS of the band border affects the dynamics of the atom even when its frequency is within the gap, giving rise to dissipation and to the failure of the perturbative approximation. This is clearly observed in figure (12.6), where in frequencies close to the band edge the dissipation observed in the results of the expansion model differs from that described within the perturbative approximation.

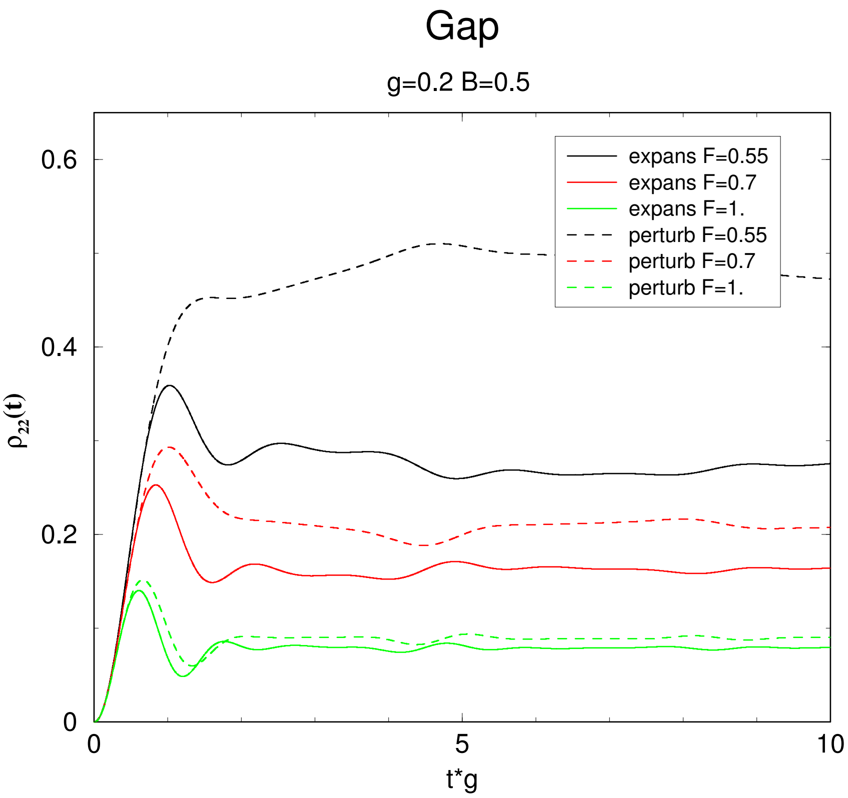

Fig. 12.6 The evolution $\sigma_z(t)$ is shown for values of F within the gap. The upper level still suffers a certain depopulation because the localization length in frequency of the photons emitted by the atom enters into the band range of frequency, having therefore a certain probability to dissipate. Because of that, they also interact with a large DOS, and that explains the failure of the perturbative approximation when the atomic rotating frequency is still nearby the band edge.

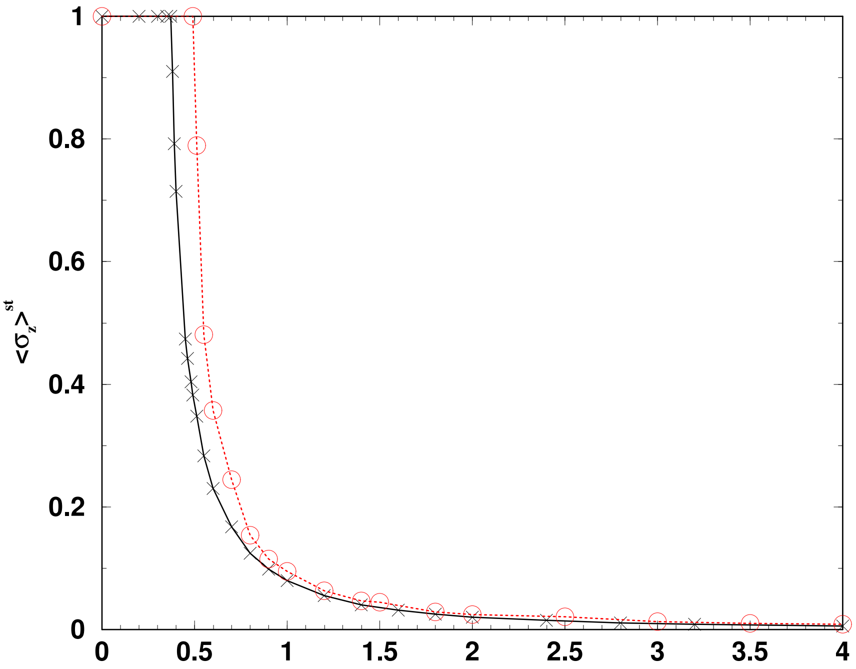

Fig. 12.7 The asymptotic value of $\sigma_z(t)$ is displayed for each value of F, both for the expansion and perturbative model. The residual long time limit population occurring at the edge of the band for the expansion model is clearly displayed. In contrast, the perturbative solution exhibits a sudden change from $\sigma_z^{st} = 1$ within the band to $\sigma_z^{st} < 1$ within the gap. The perturbative approximation becomes better (closer to the expansion model solution) when the rotating frequency is far from the band edge, no matter if it is inside the gap or the band itself.

12.3 TWO LEVEL SYSTEM DRIVEN BY AN EXTERNAL LASER FIELD.

Let us now study the effect of a single mode laser field in a two level atom, also coupled to the radiation reservoir of a photonic crystal. As in [42], we consider the interaction Hamiltonian H_{SL} of the atom with the classical coherent monochromatic laser field in the usual rotating wave approximation form [43]:

$$H_{SL} = \epsilon(\sigma_{21}e^{-i(\omega_L t+\phi_T)} + \sigma_{12}e^{i(\omega_L t+\phi_T)}), \tag{12.19}$$

where ω_L is the frequency of the laser in the coherent state $\alpha e^{-i\omega_L t}$, with $\alpha = |\alpha|e^{-i\phi_L}$. The quantity $\epsilon = \mathbf{d_{21}}\varepsilon$ is the Rabi frequency, and $|\varepsilon| = \sqrt{\omega_L/2\epsilon_0 v}\sqrt{\bar{N}_L}e_L$ the laser field magnitude, where v is the volume of the cavity, and $\bar{N}_L$ and e_L, are respectively the mean number of photons and the polarization of the laser mode. The phase ϕ_T is a global phase defined as $\phi_T = \phi_L - \pi/2$. Because of the magnitude of the laser field, the Hamiltonian H_{SL} should be considered as part of the non-interacting Hamiltonian H_0, where in this case $H_0 = H_S + H_B + H_{SL}$. We can eliminate the explicit dependence on the laser frequency by changing to a rotating frame with a frequency ω_L by using the unitary operator

$$U_t = e^{[i\omega_L t+i\phi_T][\sum_\lambda a_\lambda^\dagger a_\lambda+(\sigma_{22}-\sigma_{11})]}. \tag{12.20}$$

The rotated Hamiltonian $H' = H_0' + H_I'$,

$$\begin{aligned} H_0' &= \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda + \frac{1}{2}\omega_S\sigma_3 + \epsilon[\sigma_{21}e^{-i(\omega_L+\phi_T)} + \sigma_{12}e^{i(\omega_L t+\phi_T)}], \\ H_I' &= i\sum_\lambda g_\lambda(a_\lambda^\dagger - a_\lambda\sigma_{21}), \end{aligned} \tag{12.21}$$

can still be expressed in a simpler way by projecting it into the dressed atomic basis. The new Hamiltonian $\tilde{H} = V^{-1}H'V$, where

$$V = \begin{pmatrix} \mathbf{c} & -\mathbf{s} \\ \mathbf{s} & \mathbf{c} \end{pmatrix}, \tag{12.22}$$

will be of the form (11.6). The constants appearing in the unitary transformation matrix V are $\mathbf{c} = \cos\phi$ and $\mathbf{s} = \sin\phi$, where the angle, ϕ, is given by $\sin^2\phi = \frac{1}{2}[1 - sgn(\Delta_{SL})/\sqrt{\epsilon^2/\Delta_{SL}^2) + 1}]$. The frequency $\Delta_{SL} = \omega_S - \omega_L$. The non interacting dressed state Hamiltonian $\tilde{H}_0 = \tilde{H}_S + \tilde{H}_B + \tilde{H}_{SL}$ is equal to,

$$\tilde{H}_0 = \Omega R_3 + \sum_\lambda \Delta_\lambda a_\lambda^\dagger a_\lambda, \tag{12.23}$$

and the interaction Hamiltonian $\tilde{H}_I$ has the same form as in (11.6) once the interaction operator L is defined as:

$$L = \mathbf{cs}R_3 + \mathbf{c}^2R_{12} - \mathbf{s}^2R_{21}. \tag{12.24}$$

Here, $R_{ij} = |\tilde{i}\rangle\langle\tilde{j}|$ are the atomic operators defined in the dressed state basis $\{|\tilde{1}\rangle, |\tilde{2}\rangle\}$, and $R_3 = R_{22} - R_{11}$. The quantity $\Omega = [\epsilon^2 + \Delta_{SL}^2/4]^{1/2}$ is called the generalised Rabi frequency. According to (12.22), the relation between the dressed atomic operators and the bare atomic operators is the following,

$$\begin{aligned} \sigma_{12} &= \mathbf{cs}R_3 + \mathbf{c}^2R_{12} - \mathbf{s}^2R_{21} \\ \sigma_{21} &= \mathbf{cs}R_3 - \mathbf{s}^2R_{12} + \mathbf{c}^2R_{21} \\ \sigma_3 &= (\mathbf{c}^2 - \mathbf{s}^2)R_3 - 2\mathbf{cs}(R_{12} + R_{21}). \end{aligned} \tag{12.25}$$

Once we have established the Hamiltonian of the driven two level atom, let us now propose the two formulations we know to describe its evolutions, namely its non-Markovian stochastic Schrödinger equation and its non-Markovian master equation. In the dressed state basis presented above, and following its general definition (12.1), the non-convoluted stochastic equation for each component of the spinor in interaction image becomes,

$$\begin{aligned}
\frac{d|\tilde{\psi}_1(t)\rangle}{dt} &= g\hat{z}_t^*\{-\mathbf{cs}|\tilde{\psi}_1(t)\rangle + \mathbf{c}^2e^{-i2\Omega t}|\tilde{\psi}_2(t)\rangle\} \\
&+ g^2\int_0^t d\tau\hat{\alpha}(t-\tau)\{-\mathbf{c}^2\mathbf{s}^2|\tilde{\psi}_1(t)\rangle + \mathbf{cs}^3e^{-i2\Omega t}|\tilde{\psi}_2(t)\rangle \\
&+ \mathbf{sc}^3e^{i2\Omega(t-\tau)}e^{-i2\Omega t}|\tilde{\psi}_2(t)\rangle - \mathbf{s}^4e^{-i2\Omega(t-\tau)}|\tilde{\psi}_1(t)\rangle\} \qquad (12.26)\\
\frac{d|\tilde{\psi}_2(t)\rangle}{dt} &= g\hat{z}_t^*\{\mathbf{cs}|\tilde{\psi}_2(t)\rangle - \mathbf{s}^2e^{i2\Omega t}|\tilde{\psi}_1(t)\rangle\} \\
&+ g^2\int_0^t d\tau\hat{\alpha}(t-\tau)\{-\mathbf{c}^2\mathbf{s}^2|\tilde{\psi}_2(t)\rangle + \mathbf{c}^3\mathbf{s}e^{i2\Omega t}|\tilde{\psi}_1(t)\rangle \\
&- \mathbf{c}^4e^{i2\Omega(t-\tau)}|\tilde{\psi}_2(t)\rangle + \mathbf{cs}^3e^{-i2\Omega(t-\tau)}e^{i2\Omega t}|\tilde{\psi}_1(t)\rangle\}, \qquad (12.27)
\end{aligned}$$

where $\hat{\alpha}(t-\tau)$ and $\hat{z}_t^*$ are defined in (11.7) and (11.9) respectively, and $|\tilde{\psi}_i(t)\rangle$ is the stochastic i-spinor in the dressed state basis. Let us here define the relaxation time of the system, τ_R as the inverse of the largest value of the dissipative coefficients Γ_i with $\{i = 1, 2, 3\}$, appearing in the Redfield limit of eq. (12.27), which are defined as,

$$\begin{aligned}
\Gamma_1 &= \int_0^\infty d\tau\hat{\alpha}(t-\tau), \\
\Gamma_2 &= \int_0^\infty d\tau\hat{\alpha}(t-\tau)e^{i2\Omega(t-\tau)}, \\
\Gamma_3 &= \int_0^\infty d\tau\hat{\alpha}(t-\tau)e^{-i2\Omega(t-\tau)}. \qquad (12.28)
\end{aligned}$$

Due to the fact that the relaxation time of the system τ_R, is such that $1/\tau_R << 2\Omega$, we can use the secular approximation, which consists in eliminating the oscillating terms with frequencies 2Ω that appear in the dissipative terms. In fact, the secular approximation is normally performed over the master equation, but the dissipative terms from (12.27) will also appear in the master equation, so the approximation can be applied over them. In change, we shall not eliminate any of the noise terms, since the ensemble average of their contribution in the projector (namely the first and third terms of equation (5.64) of Chapter (5)), can give rise to non-secular components. Taking into account the above mentioned points, the resulting stochastic equation

$$\begin{aligned}
\frac{d|\tilde{\psi}_1(t)\rangle}{dt} &= g\hat{z}_t^*\{-\mathbf{cs}|\tilde{\psi}_1(t)\rangle + \mathbf{c}^2e^{-i2\Omega t}|\tilde{\psi}_2(t)\rangle\} \\
&+ g^2\int_0^t d\tau\hat{\alpha}(t-\tau)\{-\mathbf{c}^2\mathbf{s}^2|\tilde{\psi}_1(t)\rangle - \mathbf{s}^4e^{-i2\Omega(t-\tau)}|\tilde{\psi}_1(t)\rangle\} \qquad (12.29)\\
\frac{d|\tilde{\psi}_2(t)\rangle}{dt} &= g\hat{z}_t^*\{\mathbf{cs}|\tilde{\psi}_2(t)\rangle - \mathbf{s}^2e^{i2\Omega t}|\tilde{\psi}_1(t)\rangle\} \\
&+ g^2\int_0^t d\tau\hat{\alpha}(t-\tau)\{-\mathbf{c}^2\mathbf{s}^2|\tilde{\psi}_2(t)\rangle - \mathbf{c}^4e^{i2\Omega(t-\tau)}|\tilde{\psi}_2(t)\rangle\} \qquad (12.30)
\end{aligned}$$

gives rise to the following master equation,

$$\begin{aligned}
\frac{d\tilde{\rho}_{11}}{dt} &= -2g^2\mathbf{s}\mathbf{c}^3\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{-i2\Omega\tau}\tilde{\rho}_{21}\} - 2g^2\mathbf{s}^4\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{-i2\Omega(t-\tau)}\}\tilde{\rho}_{11} \\
&- 2g^2\mathbf{s}\mathbf{c}^3\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{i2\Omega t}\tilde{\rho}_{12}\} + 2g^2\mathbf{c}^4\int_0^t \Re\{\hat{\alpha}(t-\tau)e^{i2\Omega(t-\tau)}\}\tilde{\rho}_{22} \\
\frac{d\tilde{\rho}_{21}}{dt} &= -4g^2\mathbf{c}^2\mathbf{s}^2\int_0^t d\tau Re\{\hat{\alpha}(t-\tau)\}\tilde{\rho}_{21} \\
&+ g^2\int_0^t d\tau\hat{\alpha}(t-\tau)\{\mathbf{s}\mathbf{c}^3e^{i2\Omega t}\tilde{\rho}_{22} - \mathbf{c}^2\mathbf{s}^2e^{i2\Omega(t+\tau)}\tilde{\rho}_{12} \\
&+ \mathbf{c}\mathbf{s}^3e^{i2\Omega\tau}\tilde{\rho}_{11} - \mathbf{c}^4e^{i2\Omega(t-\tau)}\tilde{\rho}_{21}\} \\
&+ g^2\int_0^t d\tau\hat{\alpha}^*(t-\tau)\{\mathbf{s}\mathbf{c}^3e^{i2\Omega\tau}\tilde{\rho}_{22} - \mathbf{c}^2\mathbf{s}^2e^{i2\Omega(t+\tau)}\tilde{\rho}_{12} \\
&+ \mathbf{c}\mathbf{s}^3e^{i2\Omega t}\tilde{\rho}_{11} - \mathbf{s}^4e^{i2\Omega(t-\tau)}\tilde{\rho}_{21}\} \\
\frac{d\tilde{\rho}_{22}}{dt} &= -2g^2\mathbf{c}\mathbf{s}^3\int_0^t \Re\{\hat{\alpha}(t-\tau)e^{i2\Omega\tau}\tilde{\rho}_{12}\} + 2g^2s^4\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{-i2\Omega(t-\tau)}\tilde{\rho}_{11}\} \\
&- 2g^2\mathbf{c}\mathbf{s}^3\int_0^t \Re\{\hat{\alpha}(t-\tau)e^{-i2\Omega t}\tilde{\rho}_{21}\} - 2g^2\mathbf{c}^4\int_0^t \Re\{\hat{\alpha}(t-\tau)e^{i2\Omega(t-\tau)}\tilde{\rho}_{22}\},
\end{aligned} \tag{12.31}$$

where $\tilde{\rho}_{ij}(t)$ is the component $\{ij\}$ of the density matrix in the dressed basis. Some new rotating terms have appeared due to the average of some of the noise terms of $P_{ij}(t)$. We can now use again the secular approximation to obtain a much more simplified master equation,

$$\begin{aligned}
\frac{d\tilde{\rho}_{11}}{dt} &= 2g^2\mathbf{c}^4\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{i2\Omega(t-\tau)}\}\tilde{\rho}_{22} \\
&- 2g^2\mathbf{s}^4\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{-i2\Omega(t-\tau)}\}\tilde{\rho}_{11} \\
\frac{d\tilde{\rho}_{21}}{dt} &= -4g^2\mathbf{c}^2\mathbf{s}^2\int_0^t d\tau Re\{\hat{\alpha}(t-\tau)\}\tilde{\rho}_{21} \\
&- g^2\mathbf{c}^4\int_0^t d\tau\hat{\alpha}(t-\tau)e^{i2\Omega(t-\tau)}\tilde{\rho}_{21} \\
&- g^2\mathbf{s}^4\int_0^t d\tau\hat{\alpha}^*(t-\tau)e^{i2\Omega(t-\tau)}\tilde{\rho}_{21} \\
\frac{d\tilde{\rho}_{22}}{dt} &= 2g^2\mathbf{s}^4\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{-i2\Omega(t-\tau)}\}\tilde{\rho}_{11} \\
&- 2g^2\mathbf{c}^4\int_0^t d\tau\Re\{\hat{\alpha}(t-\tau)e^{i2\Omega(t-\tau)}\}\tilde{\rho}_{22}.
\end{aligned} \tag{12.32}$$

In the last equations we have dropped, for simplicity in the notation, the time dependence of the density matrix components, so that $\tilde{\rho}_{ij} \equiv \tilde{\rho}_{ij}(t)$. In what follows, we will compare the averaged results of (12.30) with the simplified master equation (12.32). It is clear that they will differ in the extra fast rotating terms appearing in the master equation (12.31). However, provided that the secular approximation is adequate in

the present case, such difference will not affect the main relaxation dynamics of the studied quantities.
Let us first settle the conditions necessary to obtain an asymptotic population inversion (i.e. $\rho_3 = \rho_{22} - \rho_{11} > 0$, in the non-dressed basis). As explained above, the self dressing of the atom produced by the laser field splits the original atomic level into dressed states giving rise to the well known Mollow triplet in the emission spectra. According to [42], it is necessary that the left Mollow component (which corresponds to transitions that depopulates the lower dressed state $\tilde{\omega}_1$), is situated inside the gap, while the other component (corresponding to transitions from $\tilde{\omega_2}$) remains in the band (see Figure (12.8) for a schematic representation of this.). Considering the two limits of the band (ω_c, ω_c') described before, this is equivalent to the following restriction:

$$\frac{B+F_L}{2} < \Omega < \frac{B-F_L}{2}, \tag{12.33}$$

where $F_L = \omega_L - A$. Due to the presence of the gap, the depopulation of the dressed state $|\tilde{1}\rangle$, will be less efficient than in $|\tilde{2}\rangle$ which remains in contact with the large photonic DOS of the band. As a consequence, the population in $|\tilde{1}\rangle$ is much larger than the atomic population in $|\tilde{2}\rangle$ in the long-time limit. Following (12.25), once we have ensured that $< R_3 >^{st} < 0$ in the long time limit, and provided that the coherences, $< R_{12} >$ and $< R_{21} >$, tend to disappear in such limit, it is necessary that $\mathbf{c}^2 < \mathbf{s}^2$ for $\sigma_3^{st} > 0$. To satisfy this condition, according to the definition of s^2 presented above, it is sufficient that $\Delta_{SL} < 0$.

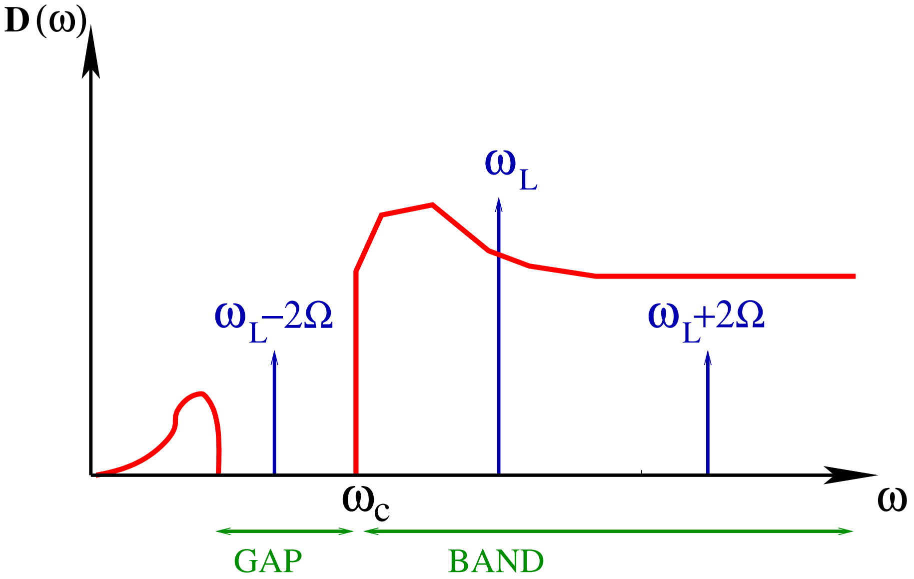

Fig. 12.8 The figure represents how the Mollow triplet should be placed with respect to the band and the gap in order to provide the necessary condition to have population inversion [42].

We must note here that $\{R_{11}, R_{22}, R_{21}, R_{12}\}$ are components of the Pauli representation of the density matrix. As shown in Appendix (Q), the element $\tilde{R}_3$ is equivalent to $\tilde{\rho}_3 = \tilde{\rho}_{22} - \tilde{\rho_{11}}$, and can therefore be calculated with the master equation (12.32).
The results shown in fig. (12.9) confirm the validity of the correlation function (11.13) for describing the behavior of the two level atom in contact with a laser and the modified EM field of the PBG. It also shows the necessity of the two conditions described above for obtaining asymptotic population inversion. We have just established that the correlation function (11.13) reproduces the same physical effects as (11.10) for a two level system within a PC and coupled to an external laser field. As we have mentioned, this correlation

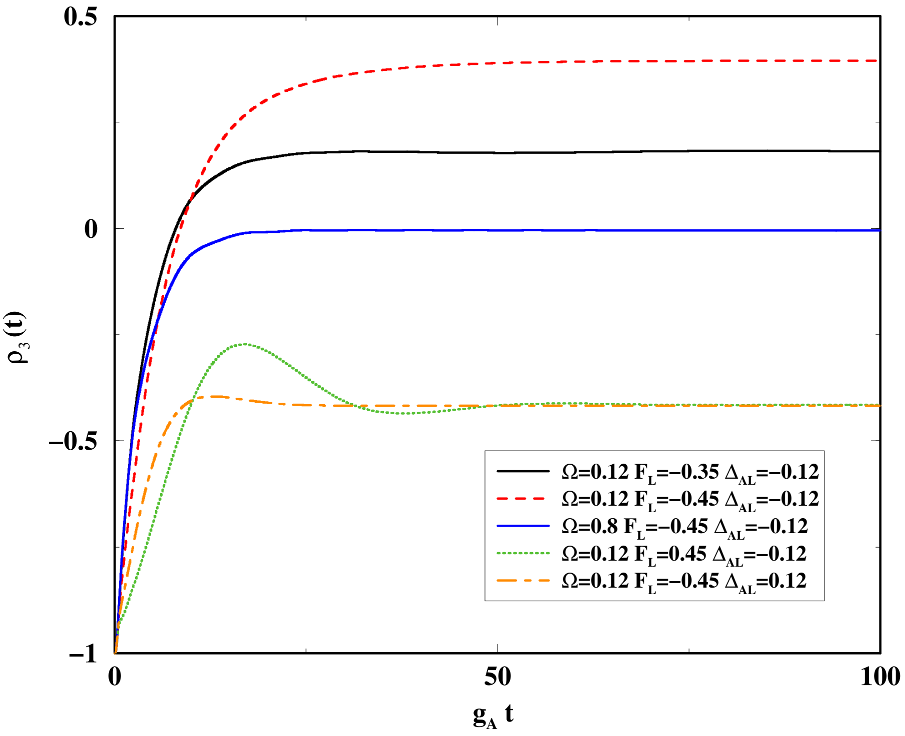

Fig. 12.9 The first two curves obey the two conditions necessary for asymptotic population inversion. Such property disappears when the condition over Ω is not satisfied (figures 3 and 4), or it is not true that $\mathbf{c}^2 > \mathbf{s}^2$ (curve 5).

function is suitable to generate the corresponding noise (see the procedure explained in Appendix (P)). Let us end this section by comparing the results of the master equation (12.32) with those of a stochastic equation such as (12.30). As clearly seen in fig. (12.10), the ensemble averaged solutions of the stochastic Schrödinger equation permit us to recover the results of the corresponding master equation. The differences observed between the two curves are due to the fast rotating terms that appear in the stochastic equation (12.30), and that have been eliminated in the master equation (12.32) through the secular approximation.

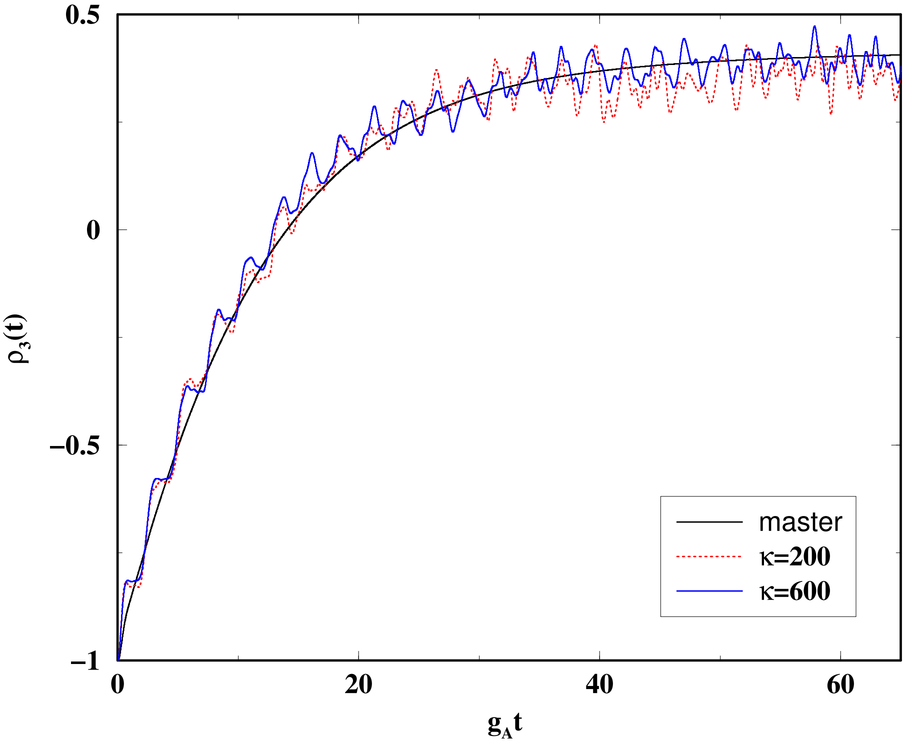

Fig. 12.10 The convergence to the average value of stochastic solutions, produced when increasing sampling or number of trajectories κ, is here displayed. As expected, such averaged value presents some additional oscillations of frequency 2Ω with respect to the master equation (12.32), due to the extra secular terms appearing in (12.31).

12.4 FLUCTUATIONS: TWO-TIME CORRELATION FUNCTIONS

Let us finish the chapter by computing the system of two-time correlation functions of a two level atom immersed in a PC. As discussed in Chapter (III), certain two-time correlations may be used to compute the atomic emission spectra. According to (9.29), the non-Markovian two-time correlation functions are given, up to second order in perturbation parameter, by the following set of differential equations,

$$\frac{d}{dt_1}\langle\Psi_0|A(t_1)B(t_2)|\Psi_0\rangle = i\langle\Psi_0|\left\{[H_S, A]\right\}(t_1)B(t_2)|\Psi_0\rangle$$

$$
\begin{aligned}
&+ \int_0^{t_1} d\tau \alpha^*(t_1-\tau)\langle\Psi_0|\left\{V_{\tau-t_1}L^\dagger[A,L]\right\}(t_1)B(t_2)|\Psi_0\rangle \\
&+ \int_0^{t_1} d\tau \alpha(t_1-\tau)\langle\Psi_0|\left\{[L^\dagger,A]V_{\tau-t_1}L\right\}(t_1)B(t_2)|\psi_0\rangle \\
&+ \int_0^{t_2} d\tau \alpha(t_1-\tau)\langle\Psi_0|\left\{[L^\dagger,A]\right\}(t_1)\left\{[B,V_{\tau-t_2}L]\right\}(t_2)|\Psi_0\rangle + \mathcal{O}(g^3). \qquad (12.34)
\end{aligned}
$$

In the following figures we display several cases of MTCF for different values of the parameter F defined in the last chapter. The parameters are $\omega_S = 1$, $g = 0.1$, and the band width $B = 0.5$. The initial state is chosen as $|\psi_0\rangle = ((1+2i)|1\rangle + (1+i)|2\rangle)/\sqrt{7}$. The intermediate time of the correlation is settled as $t_2 = 5$.

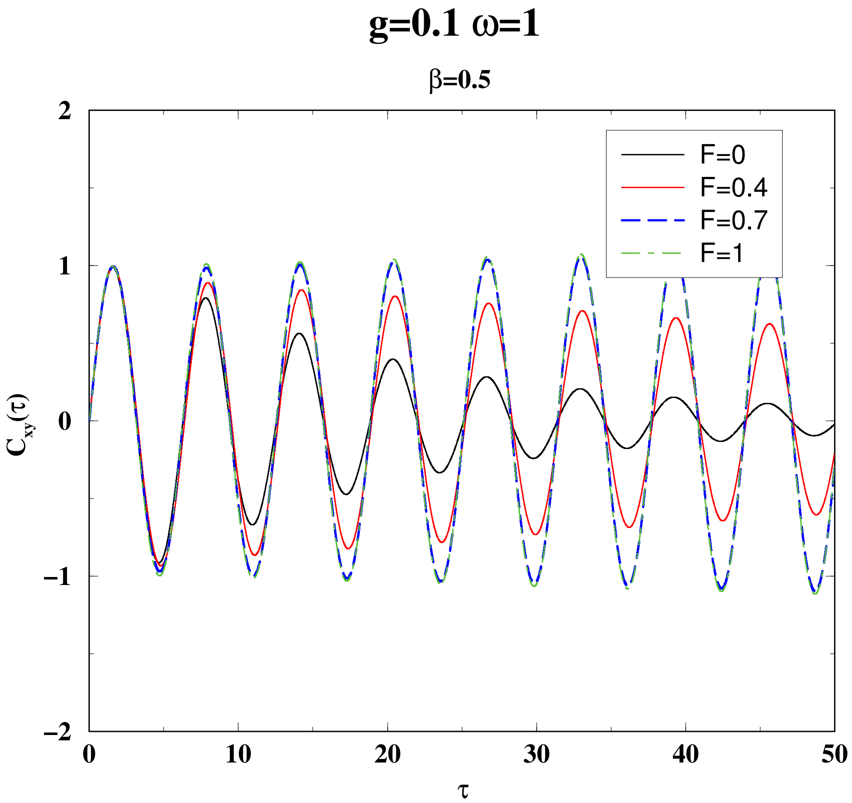

Fig. 12.11 The figure represents different values of the correlation $C_{xy} = \langle\Psi_0|\sigma_x(t_1)\sigma_y(t_2)|\Psi_0\rangle$. For values of F such that the atomic rotating frequency stays within the band, the two time correlation C_{xy} tends to vanish in the long time limit. In contrast, when $F > 0.5$ such correlation function remains always in the same value. Indeed, in the long time limit, it corresponds to $\langle\sigma_X\rangle^{asym}\langle\sigma_y(t_2)\rangle$ that does not decay to zero within the gap region.

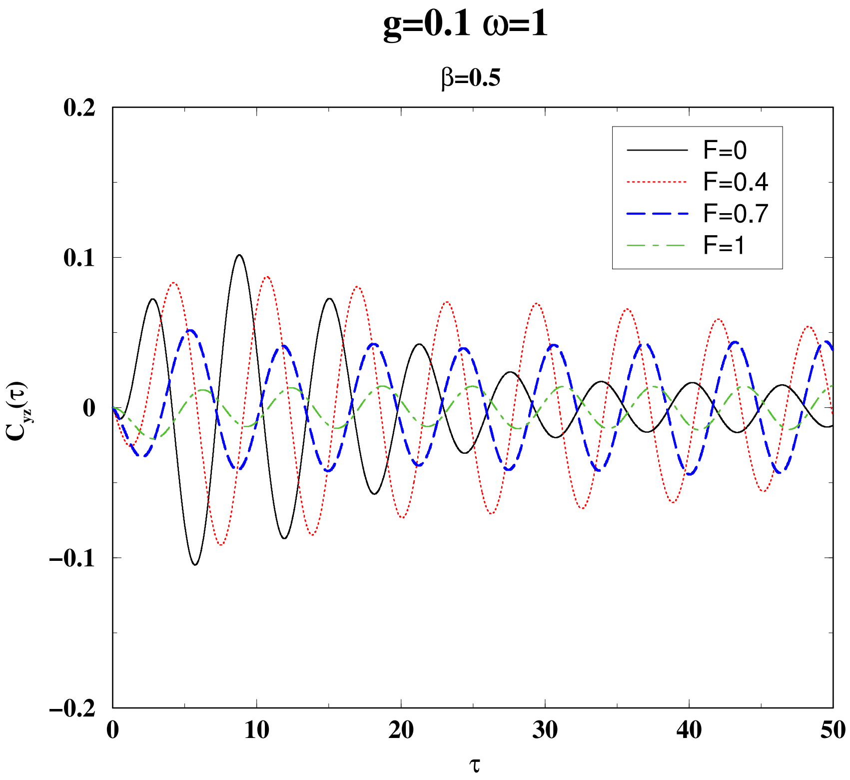

Fig. 12.12 The figure displays the correlation C_{xz}. In the long time limit (also asymptotic limit), if the rotating frequency is within the band, i.e. $F < 0.5$, the correlation tends to vanish. If it is within the gap, i.e. $F > 0.5$, it remains the same. Just as before, the asymptotic limit is $C_{xz}^{asym} \sim \langle\sigma_X\rangle^{asym}\langle\sigma_z(t_2)\rangle$. There is a qualitative difference of this curve with respect to Figure (12.11), specially for values of F within the gap: although $\langle\sigma_x\rangle^{asym}$ behaves the same for different values of F, the mean value $\langle\sigma_z(t_2)\rangle$ has different (non zero) values for each F. Hence, the curves corresponding to C_{xz} change with different values of F.

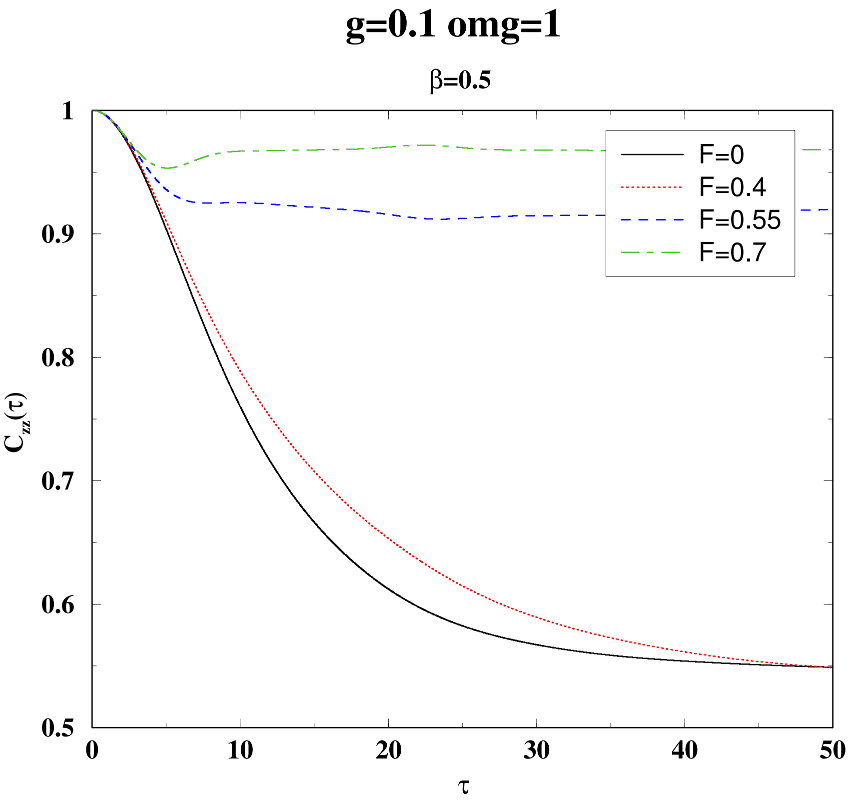

Fig. 12.13 The figure represent the correlation $C_{zz} = \langle \Psi_0 | \sigma_z(t_1)\sigma_z(t_2) | \Psi_0 \rangle$. Again, the values in the long time limit correspond to $C_{zz}^{asym} \sim \langle \sigma_z \rangle^{asym} \langle \sigma_z(t_2) \rangle$. Notice that inside the band $\langle \sigma_z \rangle^{asym} = 1$, while $\langle \sigma_z(t_2) \rangle = 0.54$ for $F = 0$, and $\langle \sigma_z(t_2) \rangle = 0.51$ for $F = 0.4$.

13

Conclusions and outlook of this part

In this part of the thesis, we have applied some of the dynamical equations developed in Parts (II) and (III) to study the dynamics of a two level atom in contact with the modified radiation field of a photonic band gap material.

As already emphasized, one of the main goals of the study is the application of the non-Markovian stochastic Schrödinger equation (12.1) to a physically realistic problem such as a two level system in contact with the radiation field of a PC. This is not only interesting on its own, but also because the steps here followed to apply stochastic equations for a two level atom (i.e. identification of Lindbland operators, generation of the correlation function and noise synthesis), can also be applied to many other physical systems. Particularly, they can be applied to many-level atoms in contact with the PBG radiation field, since the correlation function would have the same structure for any two-level transition (see for example [46]). It is in those problems where the numerical advantage of stochastic equations, in contrast with master equations, becomes evident [38]. In addition to the numerical advantage for large systems, it is important to note that if eventually a continuous measurement interpretation of non-Markovian stochastic equations is developed (analogous to the one existing for Markovian equations, see for instance [52]), this scheme might contribute to have new physical insights on the problem.

The conclusions of the work can be summarized as follows:

In Chapter (11), we characterized the radiation field with a periodic dispersion relation, instead of the parabolic dispersion relation that is used in the literature. Thanks to that, first the corresponding correlation function is non singular at the origin in contrast to the previous ones, describing more accurately the short time behavior; and second, the EM field fluctuations which correspond to the noise variable that drives the stochastic equations, can be appropriately defined.

In Chapter (12), we have shown the validity of the linear equation for the reduced propagator with $z_{i+1} = 0$ (considered as a stochastic equation), the non-convoluted master equation [1], and the new correlation function

---

[1] We note here that it was shown in Chapter (5) how the evolution equation of the reduced propagator provide an efficient tool to generate master equations. Within the second order perturbative approximation, two equivalent master equations are obtained: a non-convoluted

(11.13) to describe the dynamics of two level system in the PBG radiation field. In order to do that we have studied the physical effects observed by M. Florescu and S. John in [42] with the convoluted master equation and a radiation field characterized by a singular correlation function (11.10).

Some of the phenomena occurring in the atomic spontaneous emission were studied in Section (12.2). Indeed, when the atomic frequency ω_S is placed within the gap, we have observed asymptotic non-zero population in the excited level, together with the oscillatory behavior which is produced by the atomic self-dressing [117, 118]. For an atomic frequency placed inside the band, we have observed the non-exponential decaying of the upper level population typical of a non-Markovian interaction. In this case, we have shown that the non-convoluted master equation is more convenient than the convoluted one. While the convoluted master equation presents negative values of ρ_s for ω_S situated in the central zone of the band, the non-convoluted master equation always preserves positivity. This can be due to the fact that the stochastic equation gives rise to positive ρ_s by construction, and the non-convoluted master equation derived from it preserves this property.

The stochastic wave function $|\psi_t(z^*)\rangle$ corresponds to a measurement performed over the bath at time t that has had as a result the quantity z_t. Its evolution corresponds to a set of possible outcomes once a measurement has been performed in the environment [94]. In that sense, we have also made an attempt to qualitatively explain the behavior of single trajectories. When the atomic frequency is placed within the band, the coherences are rapidly destroyed, and the two terms of the stochastic equation, which reflect a variation of the population due to the energy interchange with the bath, are also rapidly reduced. The consequence is a large dissipation in the first time steps of each of the stochastic trajectories. Due to the rapid decrease of fluctuations, a second effect is an improvement of the sampling within the band, which means that lower number of trajectories is needed to compute the quantum mean values of system operators. In contrast, the photon-atom bound state appearing when the atomic frequency is inside the gap, gives rise to a dynamical equilibrium in which a non-zero steady state population is conserved in the upper level through the continuous emission and re-absorption of photons from the atom to the environment. In consequence, coherences are not destroyed, and for single stochastic trajectories the dissipation in energy is small, whereas the fluctuations are large and remain non-damped throughout the trajectory. Such fluctuations, which might physically occur through the continuous photon exchange between the atom and the environment, correspond to a less efficient sampling in comparison with the band case.

In Section (12.3), was shown how including the effects of a driving laser, the averaged solutions of the stochastic equation (12.30) and the master equation (12.32) describe an inversion of population under the same conditions determined by Florescu and John [42].

Finally, in Section (12.4) we have shown some of the non-Markovian two-time correlations of the atom in the PC radiation field. The calculus of two-time and four-time correlations is necessary to compute the emission spectra and photon statistics of such a system. Those are problems that remain open for future work.

master equation, equal to the one obtained in [35] by P. Gaspard and M. Nagaoka, and in [54] by Ting Yu et. al., and a convoluted master equation which corresponds to the one used by M. Florescu and S. John in [42] for the two level atom inside the photonic crystal.

Part V

CONCLUSIONS AND PERSPECTIVES

14

Conclusions

Some of the main results of this thesis are now resumed. While detailed conclusions have been discussed at the end of each part, the idea is to present here a global vision of the work.

We have studied and derived the necessary tools to describe a non-Markovian QOS linearly coupled to an environment of harmonic oscillators. As an example, we apply the equations to an atom dipolarly coupled to the radiation field within a PC.

In Part (1) the reduced propagator is introduced, an object that evolves the system state conditioned to a certain initial and final state of the environment. The reduced propagator is the matrix element of the evolution operator of the total system in the Bargmann coherent state basis for the environment. The reduced density operator, and the MTCF of the system can be expressed as a Gaussian average of reduced propagators which is performed over the different initial and final possible states. This average can be performed in two ways: First, numerically, by considering a Montecarlo sampling of the sum, so that the reduced propagators become *stochastic* propagators. Within this method, the reduced density operator and the MTCF are obtained by evolving several stochastic trajectories and then performing a sum of them. Second, analytically, so evolution equations for the density operator and the MTCF can be obtained. Concerning that issue, we have made an extension of the Novikov theorem that allows performance of the analytical average over reduced propagators with an initial state other than the vacuum.

In Part (II), particularly in Chapter (5), the sampling of several models of SSE is studied, which briefly speaking is the number of stochastic trajectories needed to obtain the reduced density operator. Particularly, we show that the non-linear type of SSEs, which are characterized by having a dynamical distribution for the noise, present an improvement of the sampling only when the environmental temperature is high enough. The reason is that it is in such condition where the environmental distribution, which coincides with the noise distribution, evolves considerably with the interaction. Afterwards, the reduced propagator is used to derive several models of master equations. We obtain a master equation suitable for arbitrary initial conditions for environment and system, and not just initially decorrelated states. By using reduced propagators, we also derive a master equation for finite temperature environments that is equal to the one obtained previously in the literature with other methods.

In Part (III) we derive a theory of non-Markovian MTCF. This part contains some of the main results of this thesis. We start by discussing two of the possible applications that MTCF may have in quantum optics, which are the calculus of the atomic emission spectra (related with a two-time correlation of field operators), and the photon statistics (related with a time-ordered two-time correlation of field operators). To this end, the relation between the correlation of field operators and the correlations of system operators is shown. Then, we derive the evolution equation of non-Markovian MTCF by using two different methods: a first one based on the use of reduced propagators, and a second one based on the use of Heisenberg equations. In Chapter (8), it is shown that when no approximations are made, the evolution equations of MTCF are organized in a hierarchy: the evolution of N-time correlations depends on $N+1$-time correlations, and successively. Although the hierarchy is not valid for computational means, it becomes useful once the dependency with higher order correlations is eliminated. This can be done by assuming some approximations. Particularly, in Chapter (9), a weak coupling approximation is used to obtain an evolucion equation of N-time correlations that do not depend on higher order correlations.

The fact that non-Markovian MTCF obey a hierarchy structure already shows that the QRT does not apply for this kind of interactions. The QRT states that in the Markovian case the evolution of N-time correlations is equal to the evolution of 1-time correlations, which is given by the master equation. Moreover, we find that even in the weak coupling limit the QRT is not fulfilled. To be more specific, in the evolution equation of N-time correlations up to second order in the perturbation parameter, some new terms appear apart from the ones of the evolution of 1-time correlations. A consequence of the latter is that for non-Markovian interactions the master equations is no longer the only equation needed to describe all the dynamical quantities of a QOS. To complete such description, and within the weak coupling limit, this equation may be complemented with the equations we propose in this thesis.

Finally, Part (IV) deals with the problem of an atom in contact with the modified radiation field within a PBG material. Along with its potential applications, this system is of interest because it presents some interesting physical phenomena due to the highly non-Markovian interaction. Such interaction is characterized by the environmental correlation function. We propose a new model of correlation function which describes the short time behavior in a more accurate way than previously existing ones. The noise corresponding to such correlation is generated in order to compute the system quantum mean values with SSE. With this scheme, some of the physical effects already described in the literature with master equations are reproduced: residual long time limit population in the excited level, existence of a photon atom bound state and long time limit population inversion when the atom is also driven by a laser. This part ends with the calculus of some two-time correlations for the system. Such quantities are needed to compute the atomic emission spectra, which connects directly with some of the perspectives of this work. But this is explained in some more detail in the next chapter.

15

Perspectives

The last two parts of the thesis, concerning MTCF and its application to atoms in PBG materials, leaves open the possibility of computing the emission spectra and photon statistics of these systems (always within the weak coupling limit).

Concerning the emission spectra, it is obvious that it may present interesting features, and due to the strongly non-Markovian character, a shape very different from the Lorentzian profile typical of Markovian interactions. It may also be interesting to study how such non-Markovian character affects the intermittent fluorescence of a three level atom immersed in a PBG material. The phenomena of intermittent fluorescence has been treated by several authors for Markovian interactions [62, 147, 148, 149, 150], and is based on an original idea of Dehmelt [145, 146] to observe single atomic transitions in an experiment. Suppose we have a three level system which consists in two excited levels $|1\rangle$ and $|2\rangle$ coupled to a common level $|0\rangle$ with a strong and a weak transition respectively. The strong transition produces a fluorescence signal that is detected. However, from time to time the electron is excited to the metastable level $|2\rangle$, and the fluorescence signal is interrupted with a dark period. Since this weak transition occurs randomly in time, the atomic fluorescence intensity has the form of a random telegraph signal [147]. In an experiment, the jump between two levels (say $|0>$ to $|2>$) can be indirectly through the appearance of a dark period in the detected signal. However, the fingerprint of intermittent fluorescence can be observed in the photon statistics [67], and in the emission spectra, that even in the Markov case is no longer a Lorentzian [67, 150]. As noted above, it would certainly be an interesting issue to observe such spectra when the three level atom is placed within a PBG, for instance by tuning the strong transition into the band, and the weak transition in the gap.

Concerning the photon statistics, particularly interesting would be the study of the photon bunching and anti-bunching effect in this kind of systems, again due to their non-Markovian behavior.

We have formally derived the evolution equation of two-time correlations for systems in a thermal environment. It may therefore be interesting to apply the equation to a particular QOS, and to compute quantities such as its emission spectra, studying how this is affected by the temperature. Computing arbitrary thermal N-time correlation functions is also possible, and does not present any qualitative difference with respect to the calculus of two-time correlations. This is also left open for future work.

It may be possible to consider a set of measurements over the non-Markovian system separated by a time interval chosen as $\Delta t > \tau_c$, in order to allow a recovering of the environment between measurements. The measurement operator acting at time $t + \Delta t$ can be chosen as a projector of $|\Psi_t\rangle = |\psi_t(z^*_{i+1})\rangle|z_{i+1}\rangle$ into the environmental state z_i, which would lead to a final state $|\Psi_{t+\Delta t}\rangle = \langle z_i|\mathcal{U}_I(t+\Delta t, t)|z_{i+1}\rangle|\psi_t(z^*_{i+1})\rangle$. Hence, the evolution produced with this kind of measurements may be described with the reduced propagators $G(z^*_i z_{i+1}|t+\Delta tt) = \langle z_i|\mathcal{U}_I(t+\Delta t, t)|z_{i+1}\rangle$. An average of this kind of trajectories may produce discrete points of the evolution of the reduced density matrix given by the master equation.

Finally, we believe that the set of evolution equations derived in this thesis may be used to compute the dynamics of some other systems displaying non-Markovian character, provided that they are linearly coupled to the environment. The possibility of applying other approximations to the evolution equation for the reduced propagator as well as the hierarchy of MTCFs is also an interesting question and a possible subject for further study.

16

Appendices

We consider $\hbar \neq 1$ in all the appendices except in the first one, since it corresponds to Chapter (1) where the model is presented.

Appendix A
Relation between gauge-dependent and gauge-independent H_I

In this appendix we first show how the Hamiltonian (1.17) is obtained from the Schrödinger equation of the free electron by imposing the local gauge invariance, i.e. the invariance of the Schrödinger equation with changes in the phase of the electronic wave function. Thereafter, is deduced the interaction Hamiltonian between electron and field in its $-\mathbf{r}\cdot\mathbf{E}(\mathbf{r},t)$ version, instead of the $-\mathbf{p}\cdot\mathbf{A}(\mathbf{r},t)$ version, described by (1.21), which is obtained by simplifying the interaction terms of (1.17).

A.1 GAUGE-INDEPENDENT HAMILTONIAN WITH $H_I \sim -\mathrm{P}\cdot\mathrm{A}(\mathrm{R},T)$

The probability of finding an electron at position $\mathbf{r}$ and time t is the same even if an arbitrary phase $\xi(\mathbf{r},t)$, even locally dependent on space and time, is added to its wave function

$$\psi(\mathbf{r},t)\rightarrow\psi(\mathbf{r},t)e^{i\xi(\mathbf{r},t)}. \tag{A.1}$$

However, the wave function (A.1) is no longer a solution of the Schrödinger equation of an electron in free motion,

$$-\frac{1}{2m}\bigtriangledown^2\psi=i\frac{\partial\psi}{\partial t}. \tag{A.2}$$

In order to satisfy local phase invariance, the motion equation of the electronic wave function should be modified with the addition of some terms

$$\left\{-\frac{1}{2m}\left[\bigtriangledown - i\frac{e}{m}\mathbf{A}(\mathbf{r},t)\right]^2 + eU(\mathbf{r},t)\right\}\psi = i\frac{\partial\psi}{\partial t}. \tag{A.3}$$

The new terms are the so-called gauge-dependent potentials $\mathbf{A}(\mathbf{r},t)$ and $U(\mathbf{r},t)$, satisfiying

$$\begin{aligned}\mathbf{A}(\mathbf{r},t) &\to \mathbf{A}(\mathbf{r},t) + \frac{1}{e}\bigtriangledown\xi(\mathbf{r},t)\\ U(\mathbf{r},t) &\to U(\mathbf{r},t) - \frac{1}{e}\frac{\partial\xi}{\partial t}(\mathbf{r},t).\end{aligned} \tag{A.4}$$

The Hamiltonian (A.3) is equal to (1.17) once it is considered the radiation Gauge, $U(\mathbf{r},t) = 0$ and $\bigtriangledown\mathbf{A}(\mathbf{r},t) = 0$, and a binding potential $V(\mathbf{r})$ is added to take into account the electrostatic potential that binds the electron to the nucleus. In that way, the steps of Section (1.2) can be followed to obtain an interaction Hamiltonian of the form $H_I \sim -\mathbf{p}\cdot\mathbf{A}(\mathbf{r},t)$.

A.2 GAUGE DEPENDENT HAMILTONIAN WITH $H_I \sim -\mathrm{R}\cdot\mathrm{E}(\mathrm{R},T)$

With the electric dipole approximation, the vector potential in an electron placed in $\mathbf{r}+\mathbf{r}_0$ (with $\mathbf{r}_0$ the position of the atomic nucleus to which it is bounded), is given by (1.26) as

$$\mathbf{A}(\mathbf{r}+\mathbf{r}_0) \sim \mathbf{A}(\mathbf{r},t)e^{i\mathbf{k}\cdot\mathbf{r}_0}, \tag{A.5}$$

so that the Schrödinger equation reads as

$$\left\{-\frac{1}{2m}\left[\bigtriangledown - i\frac{e}{m}\mathbf{A}(\mathbf{r}_0,t)\right]^2 + V(\mathbf{r},t)\right\}\psi = i\frac{\partial\psi}{\partial t}, \tag{A.6}$$

where the radiation gauge and the binding electrostatic potential has been considered. A gauge transformation to the electric field $\mathbf{E}$ can be made at this point, by defining the local phase as

$$\xi(\mathbf{r},t) = -\frac{e}{m}\mathbf{A}(t)\cdot\mathbf{r}, \tag{A.7}$$

so that we have

$$\psi(\mathbf{r},t) = e^{[ie\mathbf{A}(\mathbf{r}_0,t)\cdot\mathbf{r}]}\Psi(\mathbf{r},t), \tag{A.8}$$

which inserted in (A.6) gives rise to the following equation

$$\left[H_{el} - e\mathbf{r}\cdot\mathbf{E}(\mathbf{r}_0,t)\right]\Psi(\mathbf{r},t) = i\frac{\partial\Psi}{\partial t}. \tag{A.9}$$

Here, we have defined $H_{el} \equiv H_S$. The Hamiltonian $H_I = -\mathbf{D}\cdot\mathbf{E}(\mathbf{r}_0,t)$ should be represented in terms of the quantized electron field $\Psi(\mathbf{r},t) = \sum_j b_j\phi_j(\mathbf{r})$, with ϕ_j the eigenfunction of the electronic Hamiltonian H_{el} corresponding to the eigenvalue E_j,

$$H_I = \int d^3r\Psi^\dagger(\mathbf{r})\left[-e\mathbf{r}\cdot\mathbf{E}(\mathbf{r}_0,t)\right]\Psi(\mathbf{r}) = \mathbf{D}\cdot\mathbf{E}(\mathbf{r}_0,t) \tag{A.10}$$

Here, we have defined the dipolar moment operator as

$$\mathbf{D} = \sum_{ij} b_j^\dagger b_k \mathbf{d}_{jk}, \tag{A.11}$$

with $\mathbf{d}_{jk} = -e\int d^3r\phi_j^*(\mathbf{r})\mathbf{r}\phi_k(\mathbf{r})$. The electric field is defined as

$$\mathbf{E}(\mathbf{r}_0,t) = \sum_\lambda \epsilon_\lambda a_\lambda A_\lambda(\mathbf{r}_0)\hat{\mathbf{e}}_\lambda e^{-i\omega_\lambda t} + H.C., \tag{A.12}$$

with $\epsilon_\lambda = \sqrt{\frac{\omega_\lambda}{2\epsilon_0}}$ and $A_\lambda(\mathbf{r}_0)\hat{\mathbf{e}}_\lambda = \mathbf{A}_\lambda(\mathbf{r}_0)$ are the modes in which the field is expanded. The amplitudes $A_\lambda(\mathbf{r}_0)$ are given by (1.26). Replacing the last expression in (A.10), the interaction Hamiltonian takes the form

$$H_I = \sum_{i,j} b_j^\dagger b_k \sum_\lambda g_{\lambda,j,k}(a_\lambda + a_\lambda^\dagger), \tag{A.13}$$

with

$$g_{\lambda,j,k} = d_{jk}\sqrt{\frac{\hbar\omega_\lambda}{2\epsilon_0}}A_\lambda(\mathbf{r}_0)\mathbf{d}_{jk}\cdot\hat{\mathbf{e}}_\lambda. \tag{A.14}$$

For a two level atom, and within the rotating wave approximation (i.e. eliminating the terms in which an electron is excited (desexcited) and a photon is created (annihilated) in the field simultaneously), as well as the terms in which the dipolar coupling is forbidden (i.e. terms in which $j = k$), we have

$$H_I = \sum_\lambda \left(\sigma_{21} g_\lambda a_\lambda + \sigma_{12} g_\lambda^* a_\lambda^\dagger\right), \tag{A.15}$$

with $g_\lambda = d_{12}\sqrt{\frac{\hbar\omega_\lambda}{2\epsilon_0}}A_\lambda(\mathbf{r}_0)\hat{\mathbf{d}}_{12}\cdot\hat{\mathbf{e}}_\lambda$, and $\sigma_{jk} = b_j^\dagger b_k$.

Appendix B
Coherent states of the radiation field.

A derivation of the main properties of coherent and Bargmann coherent states is discussed in this Appendix. We follow the original presentation offered by Glauber in [48]. Some alternative ones can be found in [43, 51] or any other Quantum Optics textbook.

The radiation field is described as a sum of different harmonic oscillators λ, with Hamiltonian

$$H = \sum_{\lambda} \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}, \tag{B.1}$$

and eigenvalues $\omega_{\lambda} n_{\lambda}$, where n_{λ} is an integer, and a_{λ} and $a_{\lambda}^{\dagger}$ are the so-called annihilation and creation operators of the field for reasons that will became clear in a while. In the former Hamiltonian we have chosen the energy of the vacuum state as the energy origin [1]. In the former Hamiltonian, the energy $\frac{1}{2}\omega_{\lambda}$ is the ground state energy of the λ oscillator, also called the zero-point energy, and is often omitted for simplicity.

The state vector for the ground state of the oscillator, which we write as $|0\rangle_{\lambda}$ is defined by the condition

$$a_{\lambda}|0\rangle = 0. \tag{B.2}$$

---

[1] In fact, the theory gives us that such energy is equal to the sum $E_0 = \sum_{\lambda} \frac{1}{2}\omega_{\lambda}$, which in fact is infinite. By considering it as the origin energy, it is possible to bypass infinite quantities and calculate accurately the physical effects which are actually observable. A procedure that is known as renormalization [74].

The state vector for excited state of the oscillator may be obtained by applying integral powers of the operator $a_\lambda^\dagger$ to $|0\rangle$, for instance

$$|n_\lambda\rangle = \frac{(a_\lambda^\dagger)^{n_\lambda}}{(n_\lambda!)^{1/2}}|0\rangle;\ (n_\lambda = 0, 1, 2\cdots). \tag{B.3}$$

The former basis is the $number$ basis, which defines an environmental state with the number of photons n_λ in each mode λ. The way in which the operators a_λ and $a_\lambda^\dagger$ act upon these states is the following

$$\begin{aligned} a_\lambda|n_\lambda\rangle &= n_\lambda^{1/2}|n_\lambda - 1\rangle \\ a_\lambda^\dagger|n_\lambda\rangle &= (n_\lambda + 1)^{1/2}|n_\lambda + 1\rangle \\ a_\lambda^\dagger a_\lambda|n_\lambda\rangle &= n_\lambda|n_\lambda\rangle, \end{aligned} \tag{B.4}$$

so that the action of a_λ ($a_\lambda^\dagger$) over the number state is to annihilate (create) a photon in the mode λ. The electric field operator $E(\mathbf{r}, t)$ is separated into a positive frequency part and a negative frequency part,

$$E(\mathbf{r}, t) = E^{(+)}(\mathbf{r}, t) + E^{(-)}(\mathbf{r}, t), \tag{B.5}$$

where, as defined in Appendix (A),

$$E^{(+)}(\mathbf{r}, t) = \sum_\lambda \epsilon_\lambda a_\lambda A_\lambda(\mathbf{r})\hat{\mathbf{e}}_\lambda e^{-i\omega_\lambda t}, \tag{B.6}$$

with $\epsilon_\lambda = \sqrt{\frac{\omega_\lambda}{2\epsilon_0 v}}$ and $A_\lambda(\mathbf{r})\hat{\mathbf{e}}_\lambda = \mathbf{A}_\lambda(\mathbf{r})$ are the modes in which the field is expanded, and $E^{(-)}(\mathbf{r}, t) = \left(E^{(+)}(\mathbf{r}, t)\right)^\dagger$. It is useful to search for a basis $|\alpha_\lambda\rangle$ such that

$$E^{(+)}(\mathbf{r}, t)||\alpha_\lambda\rangle = \mathcal{E}(\mathbf{r}, t)||\alpha_\lambda\rangle, \tag{B.7}$$

where the eigenvalue functions are

$$\mathcal{E}^{(+)}(\mathbf{r}, t) = \sum_\lambda \epsilon_\lambda \alpha_\lambda A_\lambda(\mathbf{r})\hat{\mathbf{e}}_\lambda e^{-i\omega_\lambda t}, \tag{B.8}$$

so that each individual mode obeys the relation

$$a_\lambda||\alpha_\lambda\rangle = \alpha_\lambda||\alpha_\lambda\rangle. \tag{B.9}$$

This basis is known as the coherent state basis. In the next sections we discuss its relation with the number basis, as well as some of its properties. For simplicity, we may consider a single oscillator and drop the index λ

$$a||\alpha\rangle = \alpha||\alpha\rangle. \tag{B.10}$$

B.1 COHERENT STATES IN TERMS OF NUMBER STATES

Let us express the coherent state basis in terms of the complete orthonormal number basis $|n\rangle$,

$$||\alpha\rangle = \sum_n |n\rangle\langle n||\alpha\rangle, \tag{B.11}$$

where we have inserted the number state closure relation. The coefficients $\langle n|\alpha\rangle$ of the expansion can be calculated by using (B.4), and set the recurrence relations

$$\sqrt{n+1}\langle n+1||\alpha\rangle = \alpha\langle n||\alpha\rangle, \tag{B.12}$$

from which we find

$$\langle n||\alpha\rangle = \frac{\alpha^n}{(n!)^{1/2}}\langle 0||\alpha\rangle. \tag{B.13}$$

Inserting the last relation in (B.11) it follows

$$||\alpha\rangle = \langle 0||\alpha\rangle \sum_n \frac{\alpha^n}{(n!)^{1/2}}|n\rangle. \tag{B.14}$$

Imposing that the coherent state $||\alpha\rangle$ is normalized, so that $\langle\alpha||\alpha\rangle = 1$, we find that

$$\langle 0||\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}. \tag{B.15}$$

Then, the coherent state of the oscillator take the form

$$||\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_n \frac{\alpha^n}{(n!)^{1/2}}|n\rangle. \tag{B.16}$$

B.2 PROPERTIES OF COHERENT STATES

In this section we treat *some* of the properties of the coherent states, especially those that are useful for the purpose of the present work.

B.2.1 Non-orthogonality

One property of the coherent states is that two such states are not, in general, orthogonal. Let us use expression (B.16) and its complex conjugated, to find

$$\langle\alpha||\beta\rangle = e^{-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2} \sum_{n,m} \frac{(\alpha^*)^n\beta^m}{(n!m!)^{1/2}}\langle n|m\rangle, \tag{B.17}$$

which since the $|n\rangle$ are orthonormal, reduces to

$$\langle\alpha||\beta\rangle = e^{\alpha^*\beta-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\beta|^2}. \tag{B.18}$$

The absolute magnitude of the scalar product is given by

$$|\langle\alpha||\beta\rangle|^2 = e^{-|\alpha-\beta|^2}, \tag{B.19}$$

which shows that the coherent states tend to become approximately orthogonal for values of α and β which are sufficiently different.

B.2.2 Completeness

Orthogonality is a convenient property for a set of basis states but is not a necessary one. The essential property of such a set is that it should be complete. We prove this property by showing that the unit operator may be expressed as a sum or an integral, over the complex α plane, of projection operators of the form $||\alpha\rangle\langle\alpha||$. In order to describe such integrals, we introduce the differential element of area in the α plane

$$d^2\alpha = d(Re\alpha)d(Im\alpha). \tag{B.20}$$

We can also write $\alpha = |\alpha|e^{i\theta}$, so that

$$\int (\alpha^*)^n \alpha^m e^{-|\alpha|^2} d^2\alpha = \pi n! \delta_{nm}. \tag{B.21}$$

This expression, with the help of (B.16) brings the following relation,

$$\int d^2\alpha ||\alpha\rangle\langle\alpha|| = \pi \sum_n |n\rangle\langle n|, \tag{B.22}$$

which combined with the closure relation of the number states, brings the following resolution of the identity in terms of coherent states

$$\frac{1}{\pi}\int d^2\alpha ||\alpha\rangle\langle\alpha|| = 1. \tag{B.23}$$

B.2.3 Expansion of arbitrary states in terms of coherent states

As a consequence of the equation (B.23), any arbitrary state $|f\rangle$ may be expanded in terms of coherent states,

$$|f\rangle = \frac{1}{\pi}\int d^2\alpha ||\alpha\rangle f(\alpha^*) e^{-\frac{1}{2}|\alpha|^2}, \tag{B.24}$$

where

$$f(\alpha^*) = \langle\alpha||f\rangle e^{-\frac{1}{2}|\alpha|^2} \tag{B.25}$$

is an analytic function of α^*. Then, the expansion (B.24) is unique. Let us show that by taking the scalar product of both sides of such expansion with the coherent state $\langle\beta||$, and then using (B.18) to evaluate the scalar product $\langle\beta||\alpha\rangle$ to find

$$\langle\beta||f\rangle = \frac{1}{\pi} e^{-\frac{1}{2}|\beta|^2} \int d^2\alpha f(\alpha^*) e^{\beta^*\alpha - \frac{1}{2}|\alpha|^2}. \tag{B.26}$$

The function $f(\alpha^*)$ may be expanded in a convergent power series,

$$f(\alpha^*) = \sum_m c_m \frac{(\alpha^*)^m}{(m!)^{1/2}}, \tag{B.27}$$

which replaced in the integral appearing in (B.26), gives rise to the following result

$$\frac{1}{\pi}\int d^2\alpha f(\alpha^*) e^{\beta^*\alpha - \frac{1}{2}|\alpha|^2} = f(\beta^*), \tag{B.28}$$

since the integral of each member of the series

$$\frac{1}{\pi}\int d^2\alpha(\alpha^*)^m e^{\beta^*\alpha-\frac{1}{2}|\alpha|^2}=(\beta^*)^m. \tag{B.29}$$

Then, replacing (B.28) in (B.26) we find

$$f(\beta^*)=e^{\frac{1}{2}|\beta|^2}\langle\beta|f\rangle \tag{B.30}$$

which indicates the unique correspondence between the vectors $|f\rangle$ in the coefficients of their expansion $f(\alpha^*)$ in coherent states. However, for functions of both α and α^* the expansion is no longer unique. The relation (B.28), as well as

$$\frac{1}{\pi}\int d^2\alpha f(\alpha)e^{\beta\alpha^*-\frac{1}{2}|\alpha|^2}=f(\beta), \tag{B.31}$$

which is demostrated by the same means, is widely used along this thesis for the particular case of Bargmann coherent states. We show in the next section their relation with coherent states, which makes valid all the properties derived for them except for a constant factor.

B.3 BARGMANN STATES

The Bargmann coherent states are defined as [47, 48, 51]

$$|\alpha\rangle=e^{\frac{1}{2}|\alpha|^2}||\alpha\rangle=\sum_{n=0}^{\infty}\frac{\alpha^n}{(n!)^{1/2}}|n\rangle. \tag{B.32}$$

In such case, the relation (B.30) is replaced by

$$f(\beta^*)=e^{\frac{1}{2}|\beta|^2}\langle\beta|f\rangle=\langle\beta|f\rangle. \tag{B.33}$$

As mentioned above, the rest of the relations and properties (non-orthogonality, overcompleteness, and relations (B.28) and (B.31)) can be derived in the same way, just taking into account the factor $e^{\frac{1}{2}|\alpha|^2}$. The resolution of the idendity is then given by

$$1 \;=\; \frac{1}{\pi}\int d^2\alpha e^{-|\alpha|^2}|\alpha\rangle\langle\alpha|=\int d\mu(\alpha)|\alpha\rangle\langle\alpha|, \tag{B.34}$$

where we have defined the Gaussian measure as $d\mu(\alpha)=\frac{e^{-|\alpha|^2}}{\pi}$.

Appendix C
Reduced density operator

The density operator of the total system conformed by the QOS and its environment, can be defined just as $\rho_{tot} = |\Psi_t\rangle\langle\Psi_t|$, where $|\Psi_t\rangle$ is the pure state in which the total system is known to be. The reduced density matrix corresponding to the QOS is a statistical mixture, since it is expressed as

$$\rho_s(t) = Tr_B\left(\rho_{tot}(t)\right) = \int d\mu(z)|\psi_t(z^*)\rangle\langle\psi_t(z)| \tag{C.1}$$

in a continuous basis, where the function $d\mu$ represents the weight of the particular state $|\psi_t(z^*)\rangle$ in the mixture, and for a Bargmann coherent state basis is $d\mu(z) = \prod_\lambda d^2 z_\lambda \exp\left(-|z_\lambda|^2\right)$. The environment may also be expanded in a discrete basis, in which case the reduced density matrix is

$$\rho_s(t) = \sum_k P_k|\psi_{k,t}\rangle\langle\psi_{k,t}|. \tag{C.2}$$

The reduced density matrix corresponds to a statistical mixture where the precise state of the system is not known. Within a statistical mixture, the system might be with probabilities P_k in various states $|\psi_k\rangle$, which do not need to be orthogonal with each other.

C.1 POPULATIONS AND COHERENCES

The *diagonal* elements of the reduced operator, defined in the energy basis of the system, correspond to the populations appearing in the Pauli master equation described in Chapter (4). The off-diagonal terms, in change, describe the coherent part of its dynamics. For instance, in a continuous basis for the environment, and choosing a discrete basis $\{|m\rangle\}$ for the system, the populations are given by

$$\rho_{mm} = \int d\mu(z)\langle m|\psi_t(z^*)\rangle\langle\psi_t(z)|m\rangle = \int d\mu(z)|C_m(z)|^2, \tag{C.3}$$

where $|\psi_t(z^*)\rangle = \sum_m C_m(z)|\psi_0\rangle$, and therefore $|C_m(z)|^2$ is the probability that a measure over the system $|\psi_t(z^*)\rangle$ results in $|m\rangle$.

The *off-diagonal* terms are, in the same basis

$$\rho_{mp} = \int d\mu(z)\langle m|\psi_t(z^*)\rangle\langle\psi_t(z)|p\rangle = \int d\mu(z)C_m(z)C_p^*(z), \tag{C.4}$$

where now the coefficients $C_m(z)C_p^*(z)$ express the interference effects between the states $|m\rangle$ and $|p\rangle$ that can appear when $|\psi_t(z^*)\rangle$ is a coherent superposition of such states. The element ρ_{mp} is the average over such different crossing terms appearing in the statistical mixture. In contrast with the populations, ρ_{mp} can be zero even if non of the products $C_m(z)C_p^*(z)$ vanish. If $\rho_{np} = 0$, it means that the sum over z has canceled all the interference effects between $|m\rangle$ and $|p\rangle$. When $\rho_{np} \neq 0$, one can speak about a certain coherence existing between system eigenstates.

The properties of the reduced density operator are discussed in the next section, especially those such as trace preserving and positivity.

C.2 PROPERTIES OF THE DENSITY OPERATOR

The first property is that its trace is preserved during time, $Tr(\rho_s(t)) = 1$. For instance, for an initial state $\rho_{tot}(0) = |\Psi_0\rangle\langle\Psi_0|$, with $|\Psi_0\rangle = |\psi_0\rangle|0\rangle$, we have

$$\begin{aligned}
Tr\{\rho_s(t)\} &= \sum_m \langle m|\rho_s(t)|m\rangle = \int d\mu(z)\sum_m \langle m|\psi_t(z^*)\rangle\langle\psi_t(z)|m\rangle \\
&= \int d\mu(z)\langle\psi_t(z)|\psi_t(z^*)\rangle \\
&= \int d\mu(z)\langle\psi_0|\langle 0|\mathcal{U}_I^{-1}(t,0)|z\rangle\langle z|\mathcal{U}_I(t,0)|0\rangle|\psi_0\rangle \\
&= \langle\psi_0|\psi_0\rangle\langle 0|0\rangle = 1,
\end{aligned} \tag{C.5}$$

since $\mathcal{U}_I^{-1}(t,0)\mathcal{U}_I(t,0) = 1$, and $\langle\Psi_0|\Psi_0\rangle = 1$. If we have $|\Psi_0\rangle = \int d\mu(z_0)|\psi_0(z_0^*)\rangle|z_0\rangle$ then

$$Tr\{\rho_s(t)\} = \int d\mu(z_0)\int d\mu(z_0')\langle\psi_0|\psi_0\rangle\langle z_0|z_0'\rangle = 1, \tag{C.6}$$

where in the last expression we have used the property of scalar product of Bargmann states

$$\langle\alpha|\beta\rangle = e^{\alpha^*\beta}, \tag{C.7}$$

and

$$\frac{1}{\pi}\int d^2\alpha f(\alpha^*)e^{\beta^*\alpha - \frac{1}{2}|\alpha|^2} = f(\beta^*), \tag{C.8}$$

with $f(\alpha^*) = 1$.

The second property is that $\rho_s(t)$ is positive semidefinite for any given initial state.

Suppose first that the total system is initially in a pure state as defined in Section (2.2.2.1),

$$\rho_{tot}(t_0) = |\Psi_0\rangle\langle\Psi_0|, \tag{C.9}$$

with

$$|\Psi_0\rangle = \int d\mu(z_0)|\psi_0(z_0^*)\rangle|z_0\rangle, \tag{C.10}$$

and $|\Psi_0(z_0^*)\rangle = \langle\Psi_0|z_0\rangle$. Then, it was shown that the reduced density matrix is given as the mixture

$$\rho_s(t_1t_0|0) = \int d\mu(z_1)|\psi_{t_1,t_0}(z_1^*)\rangle\langle\psi_{t_1,t_0}(z_1)| \tag{C.11}$$

with $|\psi_{t_1,t_0}(z_1^*)\rangle = \int d\mu(z_0)G(z_1^*z_0|t_0t_1)|\psi_0(z_0^*)\rangle$. The former expression denotes clearly that ρ_s can be represented in a diagonal basis where all the eigenvalues are positive, provided that the measure $d\mu(z_1)$ is positive definite. It can also be proven that, for any given function $|f\rangle$, we have

$$\langle f|\rho_s(t_1t_0|0)|f\rangle = \int d\mu(z_1)|\langle f|\psi_{t_1,t_0}(z_1^*)\rangle|^2 \geq 0. \tag{C.12}$$

For an initial statistical mixture for the total state,

$$\rho_{tot}(t_0) = \int d\mu(z_0)\mathcal{J}(z_0, z_0^*)|\Psi_0(z_0^*)\rangle\langle\Psi_0(z_0)|, \tag{C.13}$$

where $\mathcal{J}(z_0, z_0^*)$ is the statistical probability for the member $|\Psi_0(z_0^*)\rangle$ of the statistical ensemble. As shown in Section (2.2.2.2), the reduced density operator is also a mixture

$$\rho_s(t_1, t_0) = \int d\mu(z_1) \int d\mu(z_0)\mathcal{J}(z_0, z_0^*)|\psi_{t_1t_0}(z_1^*z_0)\rangle\langle\psi_{t_0t_1}(z_0^*z_1)|, \tag{C.14}$$

where $|\psi_{t_1t_0}(z_1^*z_0)\rangle = G(z_1^*z_0|t_1t_0)|\psi_0(z_0^*)\rangle$. Provided that the meassure $d\mu(z)$ is positive valued, the former matrix is positive definite. Let us show that, for any given function $|f\rangle$,

$$\langle f|\rho_s(t_1, t_0)|f\rangle = \int d\mu(z_1) \int d\mu(z_0)\mathcal{J}(z_0, z_0^*)\bigg(|\langle f|\psi_{t_1t_0}(z_1^*z_0)\rangle|^2\bigg) \geq 0. \tag{C.15}$$

Appendix D
Validity of the Born approximation

In this appendix we show that the second order perturbative approximations is equivalent to assuming that $\rho_{tot}(t) = \rho_s(t) \otimes \rho_B$ during the whole evolution. This means that the Born approximation is *exact* up to second order in perturbation parameter.

Let us take equation (4.9),

$$\frac{d\rho(t)}{dt} = -\int_0^{t-t_0} d\tau Tr_B\{[V_t H_I, [V_{t-\tau} H_I, \rho_{tot}(t-\tau)]]\}, \tag{D.1}$$

which for $t_0 = 0$ is also equal to

$$\frac{d\rho(t)}{dt} = -\int_0^{t} d\tau Tr_B\{[V_t H_I, [V_{\tau} H_I, \rho_{tot}(\tau)]]\}, \tag{D.2}$$

and let us replace the Hamiltonian (4.14), so that

$$\begin{aligned}\frac{d\rho_s(t)}{dt} &= -\sum_{\gamma,\beta}\int_0^t d\tau Tr_B([V_t S_\gamma V_t B_\gamma, [V_\tau S_\beta V_\tau B_\beta, \rho_{tot}(\tau)]]) = \\ &- \sum_{\gamma,\beta}\Big\{\int_0^t d\tau V_t S_\gamma V_{-\tau} S_\beta Tr_B\left(\rho_{tot}(t) V_\tau B_\gamma V_t B_\beta\right) - V_t S_\beta Tr_B\left(\rho_{tot}(\tau) V_\tau B_\gamma V_t B_\beta\right) V_\tau S_\gamma \\ &+ \int_0^t d\tau \big(\rho_{tot}(\tau) V_t B_\beta V_\tau B_\gamma\big) V_t S_\beta V_\tau S_\gamma - V_\tau S_\gamma Tr_B\big(\rho_{tot}(t) V_t B_\gamma V_\tau B_\beta\big) V_\tau S_\beta\Big\}.\end{aligned} \tag{D.3}$$

Notice that this equation differs from (4.16) mainly in the fact that it is an *open* equation for ρ_s, and the correlations $Tr_B(\cdots)$ cannot be treated in a simple way. Let us take for instance the last one $Tr_B\left(\rho_{tot}(t) B_\gamma(t) B_\beta(\tau)\right) \equiv$

$C_{\gamma,\beta}(t,\tau)$, and express it in a Bargmann coherent state basis,

$$\begin{aligned} C_{\gamma,\beta}(t,\tau) &= \int d\mu(z_1)\int d\mu(z_1)\int d\mu(z_3)\langle z_1|z_3\rangle\mathcal{P}_\tau(z_3^*,z_1)\langle z_1|V_tB_\gamma V_\tau B_\beta|z_2\rangle = \\ &= \int d\mu(z_1)\int d\mu(z_2)\mathcal{P}_\tau(z_2^*,z_1)\mathcal{D}_{\gamma,\beta}(z_1^*,z_2) \end{aligned} \tag{D.4}$$

where $\mathcal{D}_{\gamma,\beta}(z_1^*,z_2)=\langle z_1|V_tB_\gamma V_\tau B_\beta|z_2\rangle$, $\mathcal{P}_\tau(z_2^*,z_1)=|\psi_\tau(z_2)\rangle\langle\psi_\tau(z_1)|$, and the property (see Appendix (B) of coherent states),

$$\frac{1}{\pi}\int d^2\alpha f(\alpha^*)e^{\beta^*\alpha-\frac{1}{2}|\alpha|^2}=f(\beta^*), \tag{D.5}$$

where $f(\alpha^*)$ is any function of the Bargmann state $|\alpha\rangle$, has been applied for going to the last line. The perturbative expansion of $\mathcal{P}_\tau(z_2^*,z_1)$ is, up to second order in g,

$$\begin{aligned} \mathcal{P}_\tau(z_2^*,z_1) &= \bigg\{1+\int_0^\tau ds z_{2,s}^*V_{s-\tau}L+\int_0^\tau ds\int_0^s ds' z_{2,s}^*z_{2,s'}^*V_{s-\tau}LV_{s'-\tau}L \\ &- \int_0^\tau ds\int_0^s ds'\alpha(s-s')V_{s-\tau}LV_{s'-\tau}L\bigg\}|\psi_t^0\rangle\langle\psi_t^0|\bigg\{1+\int_0^\tau ds z_{1,s}V_{s-\tau}L^\dagger \\ &+ \int_0^\tau ds\int_0^s ds' z_{1,s}z_{1,s'}V_{s'-\tau}L^\dagger V_{s-\tau}L^\dagger \\ &- \int_0^\tau ds\int_0^s ds'\alpha^*(s-s')V_{s'-\tau}L^\dagger V_{s-\tau}L^\dagger\bigg\}+\mathcal{O}(g^3). \end{aligned} \tag{D.6}$$

We now shown that the approximation $\mathcal{M}_{1,2}\left[\mathcal{P}_\tau(z_2^*,z_1)\right]=\rho_s(\tau)$ is valid only up to order g^2. In order to express the matrix element $D_{\gamma,\beta}(z_1^*,z_2)=\langle z_1|V_tB_\gamma V_\tau B_\beta|z_2\rangle$ of equation (D.4), we choose the operators defined in (1.48) of Chapter (1) as

$$B_1=\frac{1}{2}\sum_\lambda g_\lambda(a_\lambda+a_\lambda^\dagger)\,;\; B_2=\frac{i}{2}\sum_\lambda g_\lambda(a_\lambda-a_\lambda^\dagger). \tag{D.7}$$

Chosing for instance $\gamma=1$, and $\beta=2$, then we have

$$\begin{aligned} D_{12}(z_1^*,z_2) &= \frac{i}{4}\sum_{\lambda\lambda'}g_\lambda g_{\lambda'}\bigg\{z_{2,\lambda}z_{2,\lambda'}e^{-i\omega_\lambda t}e^{i\omega_{\lambda'}\tau}+z_{1,\lambda}^*z_{2,\lambda'}e^{i\omega_\lambda t}e^{i\omega_{\lambda'}\tau}-z_{1,\lambda}^*z_{2,\lambda'}e^{-i\omega_\lambda t}e^{-i\omega_{\lambda'}\tau} \\ &- \delta_{\lambda\lambda'}e^{-i\omega_\lambda t}e^{-i\omega_{\lambda'}\tau}-z_{1,\lambda}^*z_{1,\lambda'}^*e^{i\omega_\lambda t}e^{-i\omega_{\lambda'}\tau}\bigg\}. \end{aligned} \tag{D.8}$$

Equations (D.6) and (D.8), when inserted in (D.4) gives rise to

$$\begin{aligned} C_{1,2}(t,\tau) &= \frac{-i}{4}\bigg\{\alpha(t-\tau)\mathcal{M}_{1,2}\left[P_\tau^0(z_2^*,z_1)\right] \\ &+ \int_0^\tau ds\int_0^\tau ds'\Big(\alpha(\tau-s)\alpha^*(t-s')-\alpha^*(\tau-s')\alpha(t-s)\Big)V_{s-\tau}L\mathcal{M}_{1,2}\left[P_\tau^0(z_2^*,z_1)\right]V_{s'-\tau}L^\dagger \\ &- \alpha(t-\tau)\int_0^\tau ds\int_0^s ds'\Big(\alpha(s-s')V_{s-\tau}LV_{s'-\tau}L\mathcal{M}_{1,2}\left[P_\tau^0(z_2^*,z_1)\right] \end{aligned}$$

$$
\begin{aligned}
&+ \quad \alpha^*(s-s')\mathcal{M}_{1,2}\left[P^0_\tau(z_2^*,z_1)\right]V_{s'-\tau}L^\dagger V_{s-\tau}L^\dagger\Big)\\
&+ \quad \int_0^\tau ds\int_0^s ds'\Big(\alpha(t-s)\alpha(\tau-s')+\alpha(\tau-s)\alpha(t-s')\\
&+ \quad \gamma(t+\tau-(s+s'))\Big)V_{s-\tau}LV_{s'-\tau}L\mathcal{M}_{1,2}\left[P^0_\tau(z_2^*,z_1)\right]\\
&- \quad \int_0^\tau ds\int_0^s ds'\Big(\alpha^*(t-s)\alpha^*(\tau-s')+\alpha^*(\tau-s)\alpha^*(t-s')\\
&+ \quad \gamma^*(t+\tau-(s+s'))\Big)\mathcal{M}_{1,2}\left[P^0_\tau(z_2^*,z_1)\right]V_{s'-\tau}L^\dagger V_{s-\tau}L^\dagger\Big\}+\mathcal{O}(g^4)
\end{aligned}
\tag{D.9}
$$

where $\alpha(t)=\sum_\lambda g_\lambda^2\exp\left(-i\omega_\lambda t\right)$, and $\gamma(t)=\sum_\lambda g_\lambda^4 e{-}i\omega_\lambda t$. In the former equation, we have included some of the terms of $\mathcal{O}(g^4)$, but not all of them. To obtain a second order expression, only the first term of (D.9) has to be taken. Since the correlation function appearing in such term is already of second order, it is possible to replace $\mathcal{M}_{1,2}\left[P^0_\tau(z_2^*,z_1)\right]=|\psi_0\rangle\langle\psi_0|$ by $\rho_s(t)$ or even $\rho_s(\tau)$, since such replacement is correct up to zero order. However, such replacement is already not valid in the forth order terms we display in the former expression. The next coefficients can be solved in the same way, showing that the Born approximation emerges naturally from a second order expansion in the perturbative parameter.

Appendix E
Continuous measurement interpretation of Markovian SSE

In order to obtain a $trajectory$ of the system, i.e. a sequence of values of its state, it is necessary to perform a continuous measurement. However, the special feature of quantum mechanical systems is that they are disturbed by measurement. Particularly, the continuous observation of a system with von-Neumann measurements (also called *direct* measurement), gives rise to the so-called Zeno effect, which consists in a freezing of the system state [136]. For continuous monitoring of the system state, the proper measurements are the so-called $indirect$ measurements, which are based on coupling the system to an auxiliary system in which the measurement is performed. The auxiliary system is often the environment itself (the radiation field in quantum optics). Since the system is entangled with the environment, a projective measurement over the environment results in a measurement of the system state [1].

---

[1] A clarification is here in order. When we say that the state of the quantum open system is measured, it is not the state of a $single$ system, but the state corresponding to collection of these equally prepared. Let us explain this in more detail. Before the measurement, the system is represented by a reduced density matrix ρ_s, which describes a set of a large number of individual quantum systems, where each system has been prepared in a state $|\psi_t(z)\rangle$. The reduced density matrix is a mixture of such states, each of them with a particular weight $d\mu(z)$, that gives the probability in which such state appears in the mixture. For instance, when ρ_s is represented in a coherent state basis, such weight is the Gaussian measure $d\mu(z) = d^2z \exp -|z|^2/\pi$, so that

$$\rho_s = \int d\mu(z)|\psi_t(z)\rangle\langle\psi_t(z)|. \tag{E.1}$$

When a measurement with the result $z \equiv z_m$ is performed over the environment, a particular state $|\psi_t(z_m)\rangle$ is selected from the mixture. However, such state does not correspond to a single system, but rather to an ensemble of single systems equally prepared. In

The theory of indirect measurements was developed in [53, 101, 102] and present some interesting advantages with respect to direct measurements. First of all, as argued in [103], indirect measurements are more realistic than direct ones in experimental situations. Indeed, the experimenter never makes a direct measurement of the system of interest. Rather, the system of interest (the atom) interacts with its environment (the continuum of electromagnetic modes), and the experimenter observes the radiated field. Second, indirect measurements avoid the quantum Zeno paradox. This is true provided that the time difference between different measurements, i.e. the time step of the evolution, is much smaller than the correlation time of the environment. This is the case of Markovian interactions. If successive measurements are more frequent than τ_C, then we enter in the regime of the quantum Zeno effect where the possibility of spontaneous emission is significantly reduced [137]. This is one of the main reasons why it is not possible to identify the solution of non-Markovian SSE as the output of a continuous measurement experiment. This problem is treated in some more detail in next section.

The idea of considering individual solutions of a SSE as the results of a continuous measurement experiment was proposed in 1993 by H. Carmichael [52, 53]. The stochastic variable that drives a SSE is related to the result of the continuous measurement [94]. For that reason, and contrary to dynamical reduction models, continuous measurement interpretation provides reasons to determine a particular SSE or unraveling, given a certain measurement scheme [2] . According to Wiseman and Milburn [93, 103], *The relevant model of SSE for a given experimental situation depends on the method by which information is to be extracted from the light leaving the system. The state of a quantum system is always conditioned on (and in fact can be identified with) our knowledge of the system obtained from a measuring apparatus.* In this context, depending on the particular measuring device, different unravelings or stochastic trajectories are obtained.

E.1 INTERPRETATION OF NON-MARKOVIAN TRAJECTORIES

Although diffusive equations have been extended to treat non-Markovian interactions [35, 39, 40, 70, 95, 100], until now there has not been a measuring interpretation to them. Indeed, the identification of a trajectory as the result of a continuous measurement experiment relies in the fact that the state of the environment that is measured at time $t + \Delta t$ is not affected by the previous measure perfomed at time t. Since the recovering time for the measurement τ_c is finite for non-Markovian interaction, there is no interpretation of a trajectory as a sequence of continuous measurements, in which $\Delta t \rightarrow 0$. As argued by Gambetta and Wiseman in [94] all that we can say about non-Markovian SSE is that each member of the trajectory $|\psi_t(z)\rangle$ (provided that it is normalized, i.e. it is the solution of a non-linear SSE), is the state of the system conditioned on a measurement being performed at time t and yielding the result z_t (that corresponds to a certain environmental state given by $\{z_\lambda\}$). However, the linking of states at earlier times to form a trajectory is a fiction, since only in the Markovian limit a sequence of compatible measurements over the environment can be made. In that sense, it would be interesting to derive the dynamical equation that of a non-Markovian system when it is measured at time intervals $\Delta t > \tau_c$, in such a way that successive measurements do not affect each other.

---

other words, although the measurement can be performed over the environment of a *single* system (for instance an atom trapped in a quantum cavity), its result can only have statistical meaning. For instance, for a two level system the measured state can be expanded in the Hamiltonian basis as $|\psi_t(z_m)\rangle = C_1(z_m)|1\rangle + C_2(z_m)|2\rangle$. The coefficient $C_1(z_m)$ ($C_2(z_m)$) represents the probability of finding a system in the lower (upper) state, when a set of *direct* measurements is performed over such system (equally prepared for each measurement). In summary, an indirect measurement reduces the initial mixture to a particular state, but such particular state still represents an ensemble of single systems.

[2] Since a quantum system is affected by the measurement, different measurement devices will give rise to different types of trajectories. Obviously this is not the case of a classical system. Since they are not affected by the measurement, the experimental result is independent of the measurement device, except for the accuracy achieved.

We should also mention that although in the “orthodox” formulation of Quantum mechanics there is no interpretation of non-Markovian trajectories, it has been recently proposed in [139] that such interpretation exists within the hidden-variable formulation.

Finally, the idea in [81] of embedding the quantum open system in an auxiliary three level system, permits the construction of Markovian quantum trajectories for the state vector $|\Phi_t\rangle$ of the total system (system of interest, auxiliary system and environment). The idea is that the quantum jumps occurring in the total system may produce either the emission or an absorption of a *virtual* photon in the system of interest. The fact that emission is virtual, permits the emitted photon to be reabsorbed again, since there is no detection process that destroys it. The possibility of a *revival*, or a re-gaining of energy of the system is a basic non-Markovian characteristic, instead of the typically exponential decaying process of Markovian interactions.

Appendix F
SSE from the Feshbach projector operator technique.

In this appendix we discuss the derivation made by Gaspard and Nagaoka in [35] to derive the SSE (5.31). Further details shall be found in their paper. The evolution equation of the total system wave function, which depends on the coordinates of the system $\{x_s\}$ and the bath $\{x_b\}$, reads as follows,

$$i\frac{d\Psi_t(x_s,x_b)}{dt} = (H_S + H_B + g\sum_\beta S_\beta B_\beta)\Psi_t(x_s,x_b). \tag{F.1}$$

The interaction term is of the form (1.13) of Chapter (1), i.e. a sum over system $S_\beta = S_\beta^\dagger$ and environment $B_\beta = B_\beta^\dagger$ operators. These operators are chosen Hermitian without lost of generality, since as explained in Section (1.2.2) of Chapter (1) any H_I which is sum of system and environment operators can be expressed as a sum of system and environment Hermitian operators.

Let us consider for the environment a complete and orthonormal basis in its Hilbert space $\mathcal{H}_B$

$$\begin{aligned}\{\chi_n(x_b) &= \langle x_b|n\rangle\}\\ \langle m|n\rangle &= \delta_{mn}, \sum_n |n\rangle\langle n| = I_b\end{aligned} \tag{F.2}$$

where $\chi_n(x_b)$ are the basis functions and $|n\rangle$ are the corresponding kets. We can choose, for instance, the environmental eigenfunctions

$$H_B\chi_n(x_b) = e_n\chi_n(x_b), \tag{F.3}$$

where e_n are the corresponding eigenvalues. Let us note that here the environment is not necessarily a set of harmonic oscillators. If that were the case, then the quantities e_n and $\chi_n(x_b)$ could be considered its frequencies and modes. In this basis, the total wave function $\Psi_t(x_s, x_b)$ is represented in the following manner

$$\Psi_t(x_s, x_b) = \sum_n \phi_n(x_s, t)\chi_n(x_b), \tag{F.4}$$

where $\{\phi_n(x_s, t)\}$ is the set of coefficients of such linear expansion, and are given by

$$\phi_n(x_s, t) = \int \chi_n^*(x_b)\Psi_t(x_s, x_b). \tag{F.5}$$

The $\chi_n(x_b)$ functions only depend on the environmental degrees of freedom, so that the dependency of the total wave function over the system degrees of freedom is entirely encoded in the coefficients $\phi_n(x_s, t)$ of the linear decomposition. These coefficients are therefore function of the coordinates x_s and the time.

F.1 INTERPRETATION OF $\phi_N(X_S, T)$

The coefficients $\phi_n(x_s, t)$ are not normalized: only the total wave function $\Psi_t(x_s, x_b)$ is normalized. Nevertheless, their norm can be considered as the probability for the environment to be observed in a certain state $\chi_n(x_b)$

$$p_n(t) = \int dx_s |\phi_n(x_s, t)|^2 = \|\phi_n(x_s; t)\|^2. \tag{F.6}$$

In order to give a more complete interpretation, let us consider the quantum mean value of a system observable A over a certain state of the total system,

$$\begin{aligned}
\langle\Psi|A|\Psi\rangle &= \int dx_s dx_b \Psi^* A_s \Psi \\
&= \sum_{mn} \int dx_s \phi_m^* A \phi_n \int dx_b \chi_n^* \chi_m \\
&= \sum_n \int dx_s \phi_m^* A \phi_n & \text{(F.7)} \\
&= \sum_n \langle\phi_n|A|\phi_n\rangle, & \text{(F.8)}
\end{aligned}$$

where we have used the orthonormality relations (F.2) of the environmental functions. The quantum mean value of an observable of the system can be expressed as a mean over a statistical mixture represented by a reduced density matrix,

$$\rho_s = \sum_n |\phi_n\rangle\langle\phi_n|, \tag{F.9}$$

which evolves through the temporal dependency of the coefficients ϕ_λ

$$\langle x_s|\rho_s(t)|x_s'\rangle = \sum_n \phi_n(x_s; t)\phi_n(x_s; t). \tag{F.10}$$

These coefficients, once they are normalized as

$$\hat{\phi}_n(x_s;t) = \phi_n(x_s;t)/\|\phi_n(x_s;t)\|, \tag{F.11}$$

can then be considered as a statistical set of wave functions of the system. In term of such functions, the equation (F.9) can be expressed as

$$\rho_s = \sum_n p_n(t)|\hat{\phi}_n\rangle\langle\hat{\phi}_n|. \tag{F.12}$$

The statistical character of $\hat{\phi}_n(x_s;t)$ appears through its dependency on the environmental state (of index n). Then, the probability of each system wave function is given by the probability (F.6) of observing the environment in the corresponding basis state $\chi_n(x_b)$. Thus, the quantum system can no longer be described through a single wave function, but through a collection of them. Because of the entanglement, the dynamics of the system is conditioned on the dynamics of its environment.

F.2 EVOLUTION EQUATIONS FOR THE COEFFICIENTS $\{\phi_N(X_S,T)\}$

The next step is to find the evolution equation for the coefficients $\{\phi_n(x_s,t)\}$. This is done by inserting the decomposition (F.4) in the Schrödinger equation (F.1). Taking the scalar product on both side of each of the basis function $\chi(x_b)$ and using their orthonormality relation, a set of coupled differential equations is obtained,

$$\begin{aligned} i\frac{d\phi_m(x_s,;t)}{dt} &= H_S\phi_m(x_s,;t) + e_m\phi_m(x_s,;t) \\ &+ g\sum_\beta\sum_n\langle m|B_\beta|n\rangle S_\beta\phi_n(x_s,;t). \end{aligned} \tag{F.13}$$

This system of equations is not stochastic. However, the different coefficients $\phi_n(x_s,t)$ behave in a random way due to their mutual influence during the evolution through the matrix elements $\langle m|B_\beta|n\rangle$, and also because there is a large number of them. This occurs when the environment is a bath, i.e. a large system with a large density of energy levels. Thus, since to each energy level there is a corresponding eigenfunction of the basis in the expansion (F.4), there will be a large number of such coefficients $\phi_n(x_s,t)$.

Equation (F.13) can be expressed in a simpler way in interaction image with respect to the environment and the system

$$i\frac{d\varphi_m(x_s,;t)}{dt} = g\sum_\beta\sum_n\langle m|V_tB_\beta|n\rangle V_tS_\beta\varphi_n(x_s,;t). \tag{F.14}$$

F.3 EVOLUTION EQUATION FOR A SINGLE COEFFICIENT $\phi_L(X_S,T)$: FESHBACH PROJECTION OPERATOR METHOD

In order to obtain an evolution equation for a single coefficient of (F.13), the so-called *Feshbach projection operator method* is used. Such method consists in decomposing the Schrödinger equation of the total system in two equations, using the projectors P and Q that act over the total Hilbert space. These projectors have the usual properties

$$\begin{aligned} &P^2 = P = P^\dagger,\ \ Q^2 = Q = Q^\dagger \\ &QP = PQ = 0,\ \ P + Q = I \end{aligned} \tag{F.15}$$

and in this case are chosen as

$$P = I_s \otimes |l\rangle\langle l|, \; Q = I_s \sum_{n(\neq l)} |n\rangle\langle n|, \tag{F.16}$$

where I_s is the identity in the system basis. Their effect over the total wave function Ψ is the following,

$$\begin{aligned} (P\Psi)(x_s, x_b) &= \phi_l(x_s; t)\chi_l(x_b) \\ (Q\Psi)(x_s, x_b) &= \sum_{n(\neq l)} \phi_n(x_s; t)\chi_n(x_b), \end{aligned} \tag{F.17}$$

and applied over the Schrödinger equation give rise to the following system of coupled equations

$$\begin{aligned} i\frac{dP\Psi}{dt} &= PH_{tot}P\Psi + PH_{tot}Q\Psi, \\ i\frac{dQ\Psi}{dt} &= QH_{tot}Q\Psi + QH_{tot}P\Psi. \end{aligned} \tag{F.18}$$

The solution of the second non-homogeneous equation is obtained through the constant coefficient method,

$$Q\Psi(t) = e^{-iQH_{tot}Qt}Q\Psi(0) - i\int_0^t d\tau e^{iQH_{tot}Q(\tau-t)}QH_{tot}P\Psi(\tau), \tag{F.19}$$

where $Q\Psi(0)$ is the initial condition for all the coefficients $\{\phi_n(0)\}_{n(\neq l)}$ since the initial condition $\phi_l(0)$ is given by the first equation for $P\Psi$. Replacing (F.19) in the first equation of (F.18) we get the evolution of $P\Psi(t)$

$$\begin{aligned} i\frac{dP\Psi(t)}{dt} &= PH_{tot}PP\Psi(t) + PH_{tot}Qe^{-iQH_{tot}Qt}Q\Psi(0) \\ &- i\int_0^t d\tau PH_{tot}Qe^{iQH_{tot}Q(\tau-t)}QH_{tot}PP\Psi(\tau) \end{aligned} \tag{F.20}$$

Following (F.17) the temporal dependency of $P\Psi$ is through the coefficients $\phi_l(x_s; t)$, so that the former equation can be in fact written as

$$\begin{aligned} i\frac{d\phi_l(x_s; t)}{dt} &= PH_{tot}P\phi_l(x_s; t) \\ &+ PH_{tot}Qe^{-iQH_{tot}Qt}\sum_{n(\neq l)} \phi_n(x_s; t=0)\frac{\chi_n(x_b)}{\chi_l(x_b)} \\ &- i\int_0^t d\tau PH_{tot}Qe^{iQH_{tot}Q(\tau-t)}QH_{tot}P\phi_l(x_s; \tau), \end{aligned} \tag{F.21}$$

where we have divided by $\chi_l(x_b)$ on both sides of (F.20). This equation has three well differentiated terms. The first of these represents the *free* evolution given by the Hamiltonian operator of the system H_S. The second depends on the initial condition $Q\Psi(0)$ of all the coefficients except $P\Psi$. This term will be identified later on with the *stochastic forcing* over the system due to the environmental fluctuations. The third term corresponds to the *damping* of the coefficient or wave function $P\Psi$ (or ϕ_l) due to its coupling with the other coefficients $Q\Psi$, which is produced through the interaction with the environment. Being an integral up to the actual time t, this term is responsible for the non-Markovian character of the equation.

Let us now rederive (F.20) but in total interaction image with respect to the environment and the system. We retake equation (F.14) ant consider the two possible cases $m = l$ and $m \neq l$ to get the following set of coupled differential equations,

$$\begin{aligned} i\frac{\varphi_l(x_s;t)}{dt} &= g\sum_\beta V_t S_\beta \mathbf{B}_{\beta l}(t)^\dagger \cdot \mathbf{\Phi} \\ i\frac{d\mathbf{\Phi}}{dt} &= g\mathbf{W}(t)\cdot\mathbf{\Phi} + g\sum_\beta \mathbf{B}_{\beta l}(t) V_t S_\beta \varphi_l, \end{aligned} \tag{F.22}$$

where φ_l and Φ represent respectively $P\Psi$ and $Q\Psi$ in total interaction image. The quantity Φ is a column vector that gathers all the coefficients φ_n except φ_l,

$$\mathbf{\Phi}(x_s;t) = \{\varphi_n\}_{n(\neq l)}. \tag{F.23}$$

In the equation (F.22) the following column vector and matrix has been defined

$$\begin{aligned} \mathbf{B}_{\beta l}(t) &= \{\langle m|V_t B_\beta|l\rangle\}_{m(\neq l)} \\ \mathbf{W}(t) &= [\sum_\beta \langle m|V_t B_\beta|n\rangle S_\beta]_{m,n(\neq l)}. \end{aligned} \tag{F.24}$$

Using the same procedure as the one used for the calculus of (F.20), we find the following evolution equation

$$\begin{aligned} i\frac{\varphi_l(t)}{dt} &= g\sum_\beta V_t S_\beta \mathbf{B}_{\beta l}(t)^\dagger \cdot \mathbf{U}(t)\cdot\mathbf{\Phi}(0) \\ &- ig^2\int_0^t d\tau \sum_{\beta\gamma} S_\beta \mathbf{B}_{\beta l}(t)^\dagger \cdot \mathbf{U}(t-\tau)\cdot \mathbf{B}_{\gamma l}(\tau) V_\tau S_\gamma \varphi_l(\tau), \end{aligned} \tag{F.25}$$

where an evolution operator $\mathbf{U}(t)$ has been included, that is the solution of the equation

$$i\frac{d\mathbf{U}(t)}{dt} = g\mathbf{W}(t)\cdot\mathbf{U}(t), \tag{F.26}$$

with the initial condition $\mathbf{U}(0) = \mathbf{I}$. Equation (F.25) is equivalent to (F.20) in interaction image, and therefore the interpretation of its terms is analogous: the first represents the forcing of the environment over φ_l, that depends on the time and ends up by being random in the thermodynamic limit, when the number of degrees of freedom of the environment is infinite, the second represents the system energy damping due to the interaction with the environment.

F.4 PERTURBATIVE EXPANSION IN THE COUPLING PARAMETER G

We have just derived all the equations without making use of any approximation. However, in order to have a solution of equation (F.26) that can be replaced in (F.25), we need to perform a weak coupling expansion of the evolution operator. Particularly, to get a SSE such that its mean permit us getting a second order master equation, we need to take an expansion of $\mathbf{U}(t)$ up to such order

$$\mathbf{U}(t) = \mathbf{I} - ig\int_0^t dt_1 \mathbf{W}(t_1) - g^2\int_0^t\int_0^t dt_2 \mathbf{W}(t_1)\cdot\mathbf{W}(t_2) + \mathcal{O}(g^3). \tag{F.27}$$

Inserting this result in equation (F.25) and going also up to second order, we find

$$\begin{aligned} i\frac{\varphi_l(t)}{dt} &= f_l(t) \\ &- ig^2\int_0^t d\tau \sum_{\beta\gamma} V_t S_\beta \langle l|\mathbf{B}_{\beta l}(t)\mathbf{B}_\gamma(\tau)|l\rangle V_\tau S_\gamma \varphi_l(\tau) + \mathcal{O}(g^3), \end{aligned} \tag{F.28}$$

where the forcing term is given by

$$\begin{aligned} f_l(t) &= g\sum_\beta \sum_{m(\neq l)} V_t S_\beta \langle l|V_t\mathbf{B}_\beta|m\rangle \varphi_m(0) \\ &- ig^2\int_0^t d\tau \sum_{\beta\gamma}\sum_{m(\neq l)} V_t S_\beta \langle l|\mathbf{B}_\beta(t)\mathbf{B}_\gamma(\tau)|m\rangle V_\tau S_\gamma \varphi_m(0) + \mathcal{O}(g^3) \end{aligned} \tag{F.29}$$

and we have assumed that $\langle l|B_\beta|l\rangle = 0$.

F.5 STATISTICAL TIPICALITY

In order to use the evolution equation (F.28) to derive a stochastic Schrödinger equation, it is necessary to assume that the coefficient $\varphi_l(t)$ represents statistically each of the coefficients $\varphi_n(t)$ of the decomposition (F.4) of the total wave function.

Thus, it is necessary to assume that all the coefficients evolve in a similar way, so that $\varphi_l(t)$ is a typical representative of the rest of the statistical ensemble. This hypothesis, known as statistical typicality, has been justified for systems classically chaotic, but is not necessarily valid for all the environmental state basis $\chi_l(x_b)$ chosen. However, it is reasonable to suppose that for most of the environmental basis this hypothesis is fulfilled, since it has its origins in the fact that the typical eigenfunctions of high quantum numbers are statistically irregular. The states corresponding to a high quantum number in a system with a chaotic classical analogue can be written as a superposition of plane waves, with randomly distributed amplitudes.

Thanks to statistical typicality, and following a conjecture of Berry [140], the quantum mean value of an environmental operator C, over a typical eigenstate χ_l is equivalent to a quantum mean value over a representative state of the microcanonical ensemble with the corresponding energy e_l. In addition, since on the other hand the system is large, following Srednicki [141], it can also be supposed that such mean over the state of the microcanonic ensemble is essentially equivalent to a mean over a typical state of the canonical ensemble.

As a consequence, a quantum average over a typical environmental eigenstate χ_l is approximately equal to a thermal mean at the environmental temperature,

$$\langle l|C|l\rangle \approx tr_b\frac{e^{-\beta H_B}}{Z_b} \equiv tr_b\rho_b^{eq}C, \tag{F.30}$$

where as usual $Z_b = tr_b exp(-\beta H_B)$. The temperature, given by $\beta = (K_BT)^{-1}$ [1], should be fixed for a given environmental eigenenergy e_l. The variation of environmental energy due to the interaction with the system is negligible, since such variation is vary small in comparison with its energy e_l.

---

[1] Do not confuse $\beta = (K_BT)^{-1}$ with the index.

Taking the relation (F.30), the damping term (F.28) can be written as

$$\langle l|V_t B_\beta V_\tau B_\gamma|l\rangle \approx tr_b \frac{e^{-\gamma H_B}}{Z_b} \equiv tr_b \rho_b^{eq} V_t B_\beta V_\tau B_\gamma \equiv C_{\beta\gamma}(t-\tau). \tag{F.31}$$

Thanks to the statistical typicality, we have written the damping term in a form in which it is independent of the particular choice of the coefficient $|l\rangle$, so that it only depends on a function $C_{\beta\gamma}$ that are the environmental correlation functions.

F.6 FORCING TERM AS A STOCHASTIC TERM

In order to find the typical behavior of the forcing term, it is necessary to perform a hypothesis about the initial condition of the total wave function, since such initial condition is part of the term.

It is assumed that initially the total wave function is in a pure disentangled state, in such a way that it is equivalent to a tensorial product of the initial state of the system ψ and the mixed canonical state of the environment. Thus, the mean of the operator A over such state is

$$\langle \Psi(0)|A|\Psi(0)\rangle \approx Tr[|\psi(0)\rangle\langle\psi(0)| \otimes \frac{e^{-\beta H_B}}{Z_b} A], \tag{F.32}$$

which expanding Ψ in the environmental eigenfunctions reads as follows

$$\langle \Psi(0)|A|\Psi(0)\rangle \approx \\ \sum_m \frac{e^{-\beta e_m}}{Z_b} \int dx_s \int dx_b \psi^*(x_s;0)\chi_m^*(x_b) A \chi_m(x_b)\psi(x_s;0). \tag{F.33}$$

Since the total wave function is expanded with (F.4) it can be assumed that the approximate equation (F.33) can be obtained for an initial condition such that

$$\Psi(x_s,x_b;0) \approx \psi(x_s;0) \sum_m \sqrt{\frac{e^{-\beta e_m}}{Z_b}} e^{i\theta_m} \chi_m(x_b), \tag{F.34}$$

where $\{\theta_m\}$ are a set of independent random phases that are uniformly distributed in the interval $[0,2\pi]$. Following (F.34) the initial condition of the coefficients of the decomposition of the total wave function Ψ take the following form

$$\phi_m(x_s;0) = \varphi_m(x_s;0) \approx \psi(x_s;0) \sum_m \sqrt{\frac{e^{-\beta H_B}}{Z_b}} e^{i\theta_m}, \tag{F.35}$$

which is equal to the initial condition in total interaction image. Having assumed an initial disentangled pure state, all the initial coefficients (including φ_l) has been expressed in term of the same system initial state $\psi(0)$, which permits us stablishing the following relations between them

$$\varphi_m(x_s;0) \approx \varphi_l(x_s;0) e^{-\beta(e_m-e_l)/2} e^{i(\theta_m-\theta_l)}. \tag{F.36}$$

This relation is very important for establishing a stochastic differential equation that only depends on one of the coefficients φ_l, since once it is replaced in (F.29), the forcing term becomes as follows

$$f_l(t) \qquad \approx g \sum_\beta \sum_{m(\neq l)} V_t S_\beta \langle l|V_t B_\beta|m\rangle \varphi_l(0)$$

$$e^{-\beta(e_m-e_l)/2}e^{i(\theta_m-\theta_l)} - ig^2\int_0^t d\tau \sum_{\beta\gamma}\sum_{m(\neq l)} V_t S_\beta \langle l|V_t B_\beta V_\tau B_\gamma|m\rangle$$
$$V_\tau S_\gamma \varphi_l(0) e^{-\beta(e_m-e_l)/2}e^{i(\theta_m-\theta_l)} + \mathcal{O}(g^3) \tag{F.37}$$

On the other hand, taking into account that the coefficient φ_l evolves slowly in interaction image when the coupling is weak, we can solve perturbatively (F.28) up to order g

$$\varphi_l(t) \approx \varphi_l(0) - ig\int_0^t d\tau \sum_\gamma \sum_m \langle m|V_\tau B_\gamma|m\rangle V_\tau S_\gamma \varphi_l(0) + \mathcal{O}(g^3). \tag{F.38}$$

This expression, replaced in (F.37) gives us

$$\begin{aligned} f_l(t) \quad & \approx g\sum_\beta \sum_{m(\neq l)} S_\beta \langle l|V_t B_\beta|m\rangle \\ & \varphi_l(t) e^{-\beta(e_m-e_l)/2}e^{i(\theta_m-\theta_l)} + \mathcal{O}(g^3). \end{aligned} \tag{F.39}$$

The equation (F.39) can be expressed in a simpler way as,

$$f_l(t) \approx g\sum_\beta \eta_\beta(t) S_\beta \varphi_l(t), \tag{F.40}$$

where

$$\eta_\beta(t) \equiv \sum_{m(\neq l)} \langle l|V_t B_\beta|m\rangle e^{-\beta(e_m-e_l)/2}e^{i(\theta_m-\theta_l)} \tag{F.41}$$

may be interpreted as the stochastic forcing that acts over the system due to its interaction with the environment. Such noise is characterized by taking statistical averages over the random variables from which it depends. We define the average over a certain function F as

$$\overline{F(\theta)} = \frac{1}{2\pi}\int_0^{2\pi} d\theta F(\theta). \tag{F.42}$$

The mean values of η_β, following the definition of the random phases, are zero

$$\overline{\eta_\beta(t)} = 0, \tag{F.43}$$

since for all m

$$\overline{e^{i\theta_m}} = 0. \tag{F.44}$$

For the same reason the following correlation functions are zero

$$\overline{\eta_\beta(t)\eta_\gamma(s)} = 0, \tag{F.45}$$

since for every m and n

$$\overline{e^{i\theta_m+\theta_n}} = 0. \tag{F.46}$$

However, the correlation functions

$$\overline{\eta_\beta^*(t)\eta_\gamma(\tau)} = e^{\beta e_l}\sum_n \langle l|V_\tau B_\gamma|n\rangle e^{-\beta e_n}\langle n|V_t B_\beta|l\rangle, \tag{F.47}$$

are non zero, since

$$\overline{e^{i(\theta_m-\theta_n)}} = \delta_{mn} \tag{F.48}$$

Taking into account the definition of the canonical density operator representing an environment in thermal equilibrium

$$\rho_B^{eq} = \sum_n \frac{e^{-\beta H_B}}{Z_b}|n\rangle\langle n|, \tag{F.49}$$

where Z_b is the partition function defined before, the correlation (F.47) is

$$\overline{\eta_\beta^*(t)\eta_\gamma(\tau)} = \frac{Z_b}{e^{-\beta e_l}}\langle l|V_\tau B_\gamma \rho_B^{eq} V_t B_\beta|l\rangle. \tag{F.50}$$

This correlation depends on a particular environmental eigenstate χ_l. Since a typical value has to be obtained it is necessary to perform a thermal average over such states χ_l,

$$\sum_l \frac{e^{-\beta e_l}}{Z_b}\overline{\eta_\beta^*(t)\eta_\gamma(\tau)} = Tr_b[\rho_B^{eq} V_t B_\beta V_\tau B_\gamma] = C_{\beta\gamma}(t-\tau). \tag{F.51}$$

The typical value of the noise correlations is equal to the correlation function appearing in (F.31).

On the other hand, when the environment is large enough, the noise defined in (F.41) is given by a sum over a large number of oscillating complex term, that following the central limit theorem [142], gives rise to random variables of Gaussian type. As a summary, the random variables appearing in (F.41) can be taken as Gaussian noises characterized by the mean values (F.43) and the correlation functions (F.45) and (F.51).

F.7 THE STOCHASTIC SCHRÖDINGER EQUATION M.P.F.

Assuming all the approximations made above over the equation (F.28), the following stochastic differential equation is obtained for a typical coefficient φ_l

$$\begin{aligned} i\frac{\varphi_l(t)}{dt} &= g\sum_\beta \eta_\beta(t)S_\beta\varphi l(t) \\ &- ig^2\int_0^t d\tau\sum_{\beta\gamma} C_{\beta\gamma}(t-\tau)V_t S_\beta V_\tau S_\gamma \varphi_l(\tau) + \theta(g^3). \end{aligned} \tag{F.52}$$

The following step is to obtain an evolution from a general initial condition such that the reduced density matrix is a statistical mixture

$$\rho_s(0) = \sum_k |\psi_k(0)\rangle\langle\psi_k(0)|, \tag{F.53}$$

defined in terms of the system wave functions, ψ_k, and its probabilities , $\{p_k\}$, so that $\sum_k p_k = 1$. In such a case, we can consider the following statistical set of coefficients

$$\varphi_l(t) \approx \psi_{Ik}(x_s;t)\sqrt{\frac{e^{-\beta w_l}}{Z_b}}e^{i\theta_l} \tag{F.54}$$

where l is the index appering in (F.52), k specifies the member of the statistical mixture (F.53) and the subindex I of the system wave function indicates the fact that it is interation image.

The equation (F.52) is not homogeneous in the coefficient φ_l, so that replacing in it the expression (F.54), and eliminating the factor that multiplies ψ_{Ik} on both sides, the following equation is obtained in the total interaction image

$$\begin{aligned} i\frac{d\psi_{Ik}(t)}{dt} &= g\sum_\beta \eta_\beta(t)S_\beta\psi_{Ik}(t) \\ &- ig^2\int_0^t d\tau \sum_{\beta\gamma}\beta_{\beta\gamma}(t-\tau)V_tS_\beta V_\tau S_\gamma\psi_{Ik}(\tau) + \mathcal{O}(g^3). \end{aligned} \tag{F.55}$$

Going to partial interation image with respect to the environment (with $\psi = \psi_k = e^{-iH_St}\psi_{Ik}$) we have

$$\begin{aligned} i\frac{d\psi(t)}{dt} &= H_S\psi(t) + g\sum_\beta \eta_\beta(t)S_\beta\psi(t) \\ &- ig^2\int_0^t d\tau \sum_{\beta\gamma}C_{\beta\gamma}(t-\tau)V_tS_\beta V_\tau S_\gamma\psi(\tau) + \mathcal{O}(g^3). \end{aligned} \tag{F.56}$$

In this equation, the Gaussian noises $\eta_\beta(t)$ satisfy

$$\begin{gathered} \overline{\eta_\beta(t)} = 0, \overline{\eta_\beta(t)\eta_\gamma(\tau)} = 0, \\ \overline{\eta^*_\beta(t)\eta_\gamma(\tau)} = C_{\beta\gamma}(t-\tau) = C^*_{\gamma\beta}(\tau - t). \end{gathered} \tag{F.57}$$

Appendix G
Environmental state space flow

The Husimi function $Q_t(z, z^*)$ defined in (5.43) [43, 53], corresponds to the diagonal elements of the density matrix of the environment in the coherent state basis, which is given as

$$\begin{aligned} \rho_B(t) &= Tr_S\left(|\Psi_t\rangle\langle\Psi_t|\right) \\ &= \int f\mu(z) \int d\mu(z')\langle\psi_t(z)|\psi_t(z^{*'})\rangle|z\rangle\langle z'|, \end{aligned} \tag{G.1}$$

so that

$$Q_t(z, z^*) = \int d\mu(z)\langle z|\rho_B(t)|z\rangle. \tag{G.2}$$

The $|z\rangle$ are wave packets well localized in position q and momentum p around points in the phase space given by $z = (q + ip)/\sqrt{2}$. Hence the Husimi function can be considered as a quantum distribution in the phase space of the environmental degrees of freedom, that additionally have all the properties of a classical distribution function.

A very important property of the Husimi function is that its evolution equation is closed. From (5.42), it can be written as

$$\partial_t Q_t(z, z^*) = Q_0(z, z^*)[(\partial_t\langle\psi_t(z^*)|)|\psi_t(z^*)\rangle + \langle\psi_t(z^*)|(\partial_t|\psi_t(z^*)\rangle)] \tag{G.3}$$

that taking into account the linear SSE and its complex conjugate is,

$$\partial_t Q_t(z, z^*) = -g\sum_\lambda \partial_{z^*_\lambda}[ig_\lambda e^{-i\omega_\lambda t}\langle L^\dagger\rangle_t Q_t(z, z^*)] - c.c. \tag{G.4}$$

where $\langle L^\dagger \rangle_t = \langle \psi_t(z^*)|L^\dagger|\psi_t(z^*)\rangle / \langle \psi_t(z^*)|\psi_t(z^*)\rangle$ and $c.c.$ means the complex conjugate. Since only first order derivatives appear, the evolution is formally a Liouville equation, with a phase space flow given by

$$\partial_t z_\lambda^* = igg_\lambda e^{-i\omega_\lambda t}\langle L^\dagger \rangle. \tag{G.5}$$

which is equation (5.46).

Appendix H
The non-linear equations

H.1 NON LINEAR EQUATIONS FOR THE VACUUM REDUCED PROPAGATOR $G(T0|Z^*0)$

Linear equations present the problem of being rigid: no matter how the dynamics goes on, there will always be a very high probability of obtaining in the sampling vectors $z^* = (z_1^*, z_2^*, \cdots z_\lambda^* \cdots)$ with $|z|$ small. To avoid such problem, it is necessary to generate a dynamical equation that takes into account the environmental dynamics as a result of the interaction. This is done by generating a basis of time-dependent coherent states $|z^*(t)\rangle$ distributed according to the Husimi function $Q_t(z_0, z_0^*)$. Such function is defined in (5.47) as,

$$Q_t(z, z^*) = \int \frac{d^2 z_0}{\pi} Q_0(z_0, z_0^*) \delta^2(z^* - z^*(t)), \tag{H.1}$$

with the notation $\delta^2(z^* - z^*(t)) = \prod_\lambda \delta(Re(z_\lambda^* - z_\lambda^*(t)))\delta(Im(z_\lambda^* - z_\lambda^*(t)))$. When the flux (5.46) is integrated, we obtain that the eigenvalues of the environmental modes, evolving in time with the interaction have the form

$$z_\lambda^*(t) \equiv \tilde{z}_t^* = z_\lambda^*(0) + g \int_0^t d\tau g_\lambda e^{-i\omega_\lambda \tau} \langle L^\dagger \rangle, \tag{H.2}$$

where $z_\lambda^*(0) \equiv z_\lambda^*$, equals to the eigenvalues distributed according with $Q_0(z^*, z)$. In terms of (H.2), the vector $z^*(t) = (z_1^*(t), z_2^*(t), \cdots z_\lambda^*(t) \cdots)$. According to (H.1) and (H.2), one can either integrate the solutions of the linear equation $\psi_t(z^*)\rangle$ by sampling the $z^* = (z_1^*, z_2^* \cdots z_\lambda^* \cdots)$ according to $Q_t(z, z^*)$, or sample $z = (z_1^*, z_2^* \cdots z_\lambda^* \cdots)$ over $Q_0(z, z^*)$ and construct the new eigenvalues with (H.2). Obviously, the last possibility is easier to compute, since it is possible to derive the corresponding noise (referred as *shifted* *noise*) of (5.49) by replacing (H.2) in (5.12),

$$z_t^*(t) \equiv \tilde{z}_t^* = z_t^* + g\int_0^t d\tau\alpha(t-\tau)\langle L^\dagger\rangle_\tau. \tag{H.3}$$

H.1.1 Non-linear shifted equation.

Let us now derive the solutions $|\psi(\tilde{z}_t^*)\rangle$ which depend on the shifted noise $\tilde{z}_t^*$ defined in (5.49). From (5.11), we get

$$\begin{aligned} \frac{\partial}{\partial t}|\psi(z^*(t))\rangle &= \frac{\partial}{\partial t}|\psi_t(z^*(t))\rangle|_{z_t^*=\tilde{z}_t^*} + \sum_\lambda \frac{dz_\lambda^*}{dt}\frac{\partial}{\partial z_\lambda^*}|\psi_t(z_t^*)\rangle|_{z_t^*=\tilde{z}_t^*} \\ &= \frac{\partial}{\partial t}|\psi_t(z^*(t))\rangle|_{z_t^*=\tilde{z}_t^*} + i\sum_\lambda g e^{-i\omega_\lambda t}\langle L^\dagger\rangle_t \frac{\partial}{\partial z_\lambda^*}|\psi_t(z^*(t))\rangle \end{aligned} \tag{H.4}$$

where in the second line we have replaced the evolution equation (5.46) for the shifted state vectors $z^*(t)$. In the last term a derivative $\partial/\partial z_\lambda^*$ appears, which can be treated with the functional chain rule as $\frac{\partial}{\partial z_\lambda^*} = \int d\tau \frac{\partial z_\tau^*}{\partial z_\lambda^*}\frac{\delta}{\delta z_\tau^*}$. Thus, the SSE which evolves according to the shifted noise $\tilde{z}_t^*$ is

$$\begin{aligned} \frac{d}{dt}|\psi_t(z^*(t))\rangle &= (-iH_S + gL\tilde{z}_t^* - g^2L^\dagger\bar{O}(t,z^*))|\psi_t(z^*(t))\rangle \\ &+ g^2\langle L^\dagger\rangle_t\bar{O}(t,z^*)|\psi_t(z^*(t))\rangle \\ &= (-iH_S + gL\tilde{z}_t^* - g^2(L^\dagger - \langle L^\dagger\rangle)\bar{O}(t,\tilde{z}^*))|\psi_t(z^*(t))\rangle. \end{aligned} \tag{H.5}$$

H.1.2 Non-linear normalized equation.

Thanks to the new time-dependent statistical distribution, we can define the reduced density matrix in terms of normalized wave functions, $|\tilde{\psi}_t\rangle$, as

$$\begin{aligned} \rho_s(t) &= \int d^2z Q_t(z,z^*)\frac{|\psi_t(z^*)\rangle\langle\psi_t(z^*)|}{\langle\psi_t(z^*)|\psi_t(z^*)\rangle} \\ &= \int d^2z Q_t(z,z^*)|\tilde{\psi}_t(z^*)\rangle\langle\tilde{\psi}_t(z^*)| \end{aligned} \tag{H.6}$$

where $|\tilde{\psi}_t(z^*)\rangle = |\psi_t(z^*)\rangle/\sqrt{\langle\psi_t(z^*)|\psi_t(z^*)\rangle}$. The evolution equation for these normalized wave functions can be calculated by following an analogous procedure as the former one. That is

$$\begin{aligned} \frac{d}{dt}|\tilde{\psi}_t(z^*(t))\rangle &= \frac{1}{\sqrt{\langle\psi_t(z^*)|\psi_t(z^*)\rangle}}\frac{d}{dt}|\psi(z^*(t))_t\rangle \\ &+ (\frac{d}{dt}\frac{1}{\sqrt{\langle\psi_t(z^*)|\psi_t(z^*)\rangle}})|\psi(z^*(t))_t\rangle, \end{aligned} \tag{H.7}$$

which eliminating certain time-dependent global phases, give rise to the following equation for $|\tilde{\psi}_t(z^*(t))\rangle$,

$$\begin{aligned} \frac{d}{dt}|\tilde{\psi}_t(z^*(t))\rangle &= -iH|\tilde{\psi}_t(z^*(t))\rangle + g(L - \langle L^\dagger\rangle)\tilde{z}_t|\tilde{\psi}_t(z^*(t))\rangle \\ &- g^2[(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,z^*(t)) - \langle(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,z^*(t))]|\tilde{\psi}_t(z^*(t))\rangle, \end{aligned} \tag{H.8}$$

with $\langle L\rangle_t = \langle\tilde{\psi}_t(z^*(t))|L|\tilde{\psi}_t(z^*(t))\rangle$.

H.2 THE NON-LINEAR EQUATION FOR THE REDUCED PROPAGATOR $G(T, T_0|Z^* Z_0)$

As mentioned earlier, stochastic linear equations are good enough for describing the dynamics of an open system coupled to an environment of oscillators at low temperatures [1]. However, at high temperatures the solutions of the linear equation may lose their norm and therefore statistical relevance. This is due to the fact that, within this regime, the state distribution of the environment is changing quite dramatically because of the interaction with the system. As noted in [40], the solution is to change such distribution to a time-dependent one through a Girsanov transformation. Following their procedure, we define the time-dependent distribution as,

$$\begin{aligned} Q_{t_1,t_0}(z_0, z_0^*; z_1, z_1^*) &= \frac{e^{-|z|^2}}{\pi} \langle z_1 | \mathrm{Tr}_{sys} \left[\mathcal{U}_I(t_1, t_0) |\psi_0\rangle |z_0\rangle \langle z_0'| \langle \psi_0 | \mathcal{U}_I^{-1}(t_1, t_0) \right] |z_1\rangle \\ &= \frac{e^{-|z_1|^2}}{\pi} \langle \psi_0 | G^{-1}(t_0 t_1 | z_0'^* z) G(t, t_0 | z^* z_0) |\psi_0\rangle \\ &= \frac{e^{-|z|^2 + z_1^* z_0 + z_0'^* z}}{\pi} \langle \psi_0 | \tilde{G}^{-1}(t_0 t_1 | z_0'^* z_1) \tilde{G}(t_1, t_0 | z_1^* z_0) |\psi_0\rangle, \end{aligned} \tag{H.9}$$

where $G(t_1, t_0|z_1^* z_0) = e^{z_1^* z_0} \tilde{G}(t_1, t_0|z_1^* z_0)$. With this distribution the density matrix is defined as,

$$\begin{aligned} \rho_t &= \int d^2 z_1 \frac{e^{-|z_1|^2}}{\pi} G(t t_0 | z_1^* z_0) |\psi_0\rangle \langle \psi_0 | G^{-1}(t_0 t_1 | z_0'^* z_1) \\ &= \int d^2 z_1 Q_{t_1,t_0}(z_0, z_0^*; z_1, z_1^*) \left\{ \frac{G(t_1 t_0 | z_1^* z_0) |\psi_0\rangle \langle \psi_0 | G^{-1}(t_0 t_1 | z_0'^* z_1)}{\langle \psi_0 | \tilde{G}^{-1}(t_0 t_1 | z_0'^* z_1) \tilde{G}(t_1 t_0 | z_1^* z_0) |\psi_0\rangle} \right\}. \end{aligned} \tag{H.10}$$

The evolution equation for the distribution $Q_{t_1,t_0}(z_1, z^*)$ is, using the definition of such function and the dissipative version of equation (7.50), the following,

$$\frac{\partial Q_{t_1,t_0}(z_0, z_0^*; z_1, z_1^*)}{\partial t_1} = \sum_\lambda \frac{\partial}{\partial z_{1,\lambda}} \left\{ i g_\lambda e^{i\omega_\lambda t_1} \langle L \rangle_{t_1 t_0} Q_{t_1,t_0}(z_0, z_0^*; z_1, z_1^*) \right\} - c.c., \tag{H.11}$$

where $\langle L \rangle_{t_1 t_0} = \frac{\langle \psi_0 | \tilde{G}^{-1}(t_1 t_0 | z_0'^*, z_1) L \tilde{G}(t_1 t_0 | z_1^* z_0) |\psi_0\rangle}{\langle \psi_0 | \tilde{G}^{-1}(t_0 t_1 | z_0^* z_1) \tilde{G}(t_1 t_0 | z_1^* z_0) |\psi_0\rangle}$. This evolution equation is formally a Liouville equation with the phase space flow,

$$\dot{z}_{1,\lambda}^* = i g_\lambda e^{i\omega_\lambda t_1} \langle L \rangle_{t_1 t_0}. \tag{H.12}$$

The next steps to arrive to a non-linear equaiton with time-dependent distribution are again analogous to those described in [40, 41]. First, a Girsanov transformation has to be performed, so that the time dependency of $Q_{t_1,t_0}(z_0, z_0^*; z_1, z_1^*)$ is translated into the noise, which now has this form,

$$\tilde{z}_{1,t} = z_{1,t} + \int_{t_0}^{t_1} d\tau \alpha(t_1 - \tau) \langle L^\dagger \rangle_{\tau t_0}. \tag{H.13}$$

This expression has been obtained considering that the coherent state eigenvalues that enters in the sum $z_{1,t} = i \sum_\lambda g_\lambda z_{1,\lambda} \exp(-i\omega_\lambda t_1)$ are, according to (H.12), $z_\lambda^*(t_1) = z_{1,\lambda}^* + i g_\lambda \int_{t_0}^{t_1} d\tau e^{-i\omega_\lambda \tau} \langle L \rangle_{\tau t_0}$. With this transformation, the density matrix can be calculated as

$$\rho_{t_1} = \int d^2 z_1 \frac{e^{-|z_1|^2}}{\pi} \frac{\tilde{G}(t_1 t_0 | z^*(t_1) z_0) |\psi_0\rangle \langle \psi_0 | \tilde{G}^{-1}(t_0 t_1 | z_0'^* z(t_1))}{\langle \psi_0 | \tilde{G}^{-1}(t_0 t_1 | z_0'^* z(t_1)) \tilde{G}(t_1 t_0 | z^*(t_1) z_0) |\psi_0\rangle} \tag{H.14}$$

The evolution equation for the double propagator $G(t|z^*(t)z_0)$, that depends on the *shifted noise*, is derived as follows,

$$\begin{aligned}\frac{d}{dt_1}\tilde{G}(t_1t_0|z_1^*z_0) &= \sum_\lambda \frac{\partial\tilde{G}(t_1t_0|z_1^*z_0)}{\partial z_{1,\lambda}^*}\frac{\partial z_{1,\lambda}^*}{\partial t_1} + \frac{\partial\tilde{G}(t_1t_0|z_1^*z_0)}{\partial t_1} \\ &= \left\{-iH_S + L\tilde{z}_{t_1}^* - L^\dagger z_{0,t_1} - \left(L^\dagger - \langle L\rangle_{t_1t_0}\right)\int_{t_0}^{t_1} d\tau\alpha(t_1-\tau)\frac{\delta}{\delta z_\tau^*}\right\}\tilde{G}(t_1t_0|z_1^*z_0).\end{aligned} \tag{H.15}$$

The main point to be noticed in this equation is the fact that only the noise corresponding to the *final* state of the bath is shifted (in this case $z_{1,t}$), while the initial one (in this case z_{0,t_1}) remains the same.

Appendix I
Novikov property

To calculate multiple time correlation functions from (7.45), or their evolution equations, it is necessary to perform averages over the environmental coordinates. The main type of average we are going to deal with is that of the product of a Gaussian noise z_{i,t_i} with any functional $\hat{\mathcal{W}}[t_i, t_{i+1}]$. From the Novikov theorem, this is equal to

$$\mathcal{M}_i\left[z_{i,t_i}\hat{\mathcal{W}}[t_i, t_{i+1}]\right] = \int_0^t d\tau \mathcal{M}_i\left[z_{i,t} z^*_{i,\tau}\right] \mathcal{M}_i\left[\left(\frac{\delta\hat{\mathcal{W}}[t_i, t_{i+1}]}{\delta z^*_{i,\tau}}\right)\right] \tag{I.1}$$

where we have settled $\int d\mu(z_i)F = \mathcal{M}_i\left[F\right]$, as defined in (2.47). For expression (I.1) to be held, it is necessary that the noise z_{i,t_i} is a Gaussian noise of zero mean, and the functional $\hat{\mathcal{W}}[t_i, t_{i+1}]$ is such that $\frac{\partial\hat{\mathcal{W}}[t_{i+1}, t_{i+1}]}{\partial z_i} = 0$. This is what we find in single evolution equations, where $\hat{\mathcal{W}}[t_i, t_{i+1}] = \langle\psi_0 \mid G^\dagger(0 z_i|t_i t_{i+1}) A_i G(z^*_i 0|0 t_i) \mid \psi_0\rangle$. However, in the calculus of evolution equations of multiple-time correlation functions (for instance equations in (8.18) and (8.23)), we will often find terms such that the functional is

$$\begin{aligned}\mathcal{W}[t_i, t_{i+1}] = \langle\psi_0 \mid G^\dagger(0 z_i|t_i t_{i+1}) A_i G(z^*_i z_{i+1}|t_i t_{i+1}) A_{i+1} G(z^*_{i+1} z_{i+2}|t_{i+1} t_{i+2}) \cdots \\ \cdots G(z^*_N z_{N+1}|t_1 t_0) \mid \psi_0\rangle\end{aligned} \tag{I.2}$$

Notice that, to simplify the notation, we have only denoted explicitly the time dependency on the domain in which the functional depends on the noise z_{i,t_i} that appears in the property (I.1), i.e. $\mathcal{W}[t_i, t_{i+1}]$. The functional (I.2) is such that $\partial\mathcal{W}[t_{i+1}, t_{i+1}]/\partial z_i = z_{i+1}$, since the initial condition of the propagator is $G(z^*_i z_{i+1}|t_{i+1} t_{i+1}) = \exp\left(z^*_i z_{i+1}\right)$. However, let us now consider that such propagator can be separated in two parts, such that

$$G(z_i^* z_{i+1}|t_i t_{i+1}) = G(z_i^* z_{i+1}|t_{i+1} t_{i+1})\hat{G}(z_i^* z_{i+1}|t_i t_{i+1}), \tag{I.3}$$

where $G(z_i^* z_{i+1}|t_{i+1} t_{i+1}) = \exp(z_i^* z_{i+1})$. Now, the propagator $\hat{G}(z_i^* z_{i+1}|t_i t_{i+1})$ has initial condition I,and its only dependence on the environmental coordinates is through the noises z^*_{i,t_i} and $z_{i+1,t_{i+1}}$. Within that notation, we set the functional (I.2) as $\mathcal{W}[t_i, t_{i+1}] = \exp(z_i^* z_{i+1})\hat{\mathcal{W}}[t_i, t_{i+1}]$. Let us now prove that, for such functional

$$\begin{aligned} \mathcal{M}_i\left[z_{i,t_i}\mathcal{W}[t_i, t_{i+1}]\right] &= z_{i+1,t_i}\mathcal{M}_i\left[\mathcal{W}[t_i, t_{i+1}]\right] \\ &+ \int_{t_{i+1}}^{t_i} d\tau \mathcal{M}_i\left[z_{i,t} z^*_{i,\tau}\right]\mathcal{M}_i\left[\left(\frac{\delta\mathcal{W}[t_i, t_{i+1}]}{\delta z^*_{i,\tau}}\right)\right]. \end{aligned} \tag{I.4}$$

Let us start from the last term of the right hand side,

$$\begin{aligned} &\int_{t_{i+1}}^{t_i} d\tau \mathcal{M}_i\left[z_{i,t} z^*_{i,\tau}\right]\mathcal{M}_i\left[\left(\frac{\delta\mathcal{W}[t_i, t_{i+1}]}{\delta z^*_{i,\tau}}\right)\right] \\ &= \int d^2 z_i \int_0^t d\tau Q(z_i^*, z_{i+1})\alpha(t_i - \tau)\left(\frac{\delta\hat{\mathcal{W}}[t_i, t_{i+1}][z^*_{i,t_i}, z_{i+1,t_{i+1}}]}{\delta z^*_{i,\tau}}\right) \end{aligned} \tag{I.5}$$

where in the second line we have included the initial condition of (I.3), which is included in $\mathcal{W}[t_i, t_{i+1}]$, in the function $Q(z_i^*, z_{i+1}) = \exp(-z_i^* z_i)\exp(z_i^* z_{i+1})$. The average $\mathcal{M}_i\left[z_{i,t} z^*_{i,\tau}\right] = \alpha(t_i - \tau)$. From the functional chain rule, we know that

$$\frac{\partial}{\partial z^*_\tau} = \int d\tau \frac{\partial z^*_\tau}{\partial z^*_\lambda}\frac{\delta}{\delta z^*_\tau} = \int d\tau(-ig_\lambda e^{i\omega_\lambda \tau})\frac{\delta}{\delta z^*_\tau} \tag{I.6}$$

where the second line has been obtained by using (7.47). Replacing the last expression in (I.5), we obtain the following expression

$$\begin{aligned} &\int d^2 z_i Q(z_i^*, z_{i+1})\int_0^t d\tau \alpha(t_i - \tau)\left(\frac{\delta\mathcal{W}[t_i, t_{i+1}]}{\delta z^*_{i,\tau}}\right) \\ &= \int d^2 z_i Q(z_i^*, z_{i+1})\sum_\lambda i g_\lambda e^{-i\omega_\lambda t_i}\frac{\partial}{\partial z^*_{i,\lambda}}\hat{\mathcal{W}}[t_i, t_{i+1}]. \end{aligned} \tag{I.7}$$

Integrating by parts the last expression, we find that (I.5) is equal to

$$\begin{aligned} &\int_{t_{i+1}}^{t_i} d\tau \mathcal{M}_i\left[z_{i,t} z^*_{i,\tau}\right]\mathcal{M}_i\left[\left(\frac{\delta\mathcal{W}[t_i, t_{i+1}]}{\delta z^*_{i,\tau}}\right)\right] \\ &= \int d^2 z_i Q(z_i^*, z_{i+1})\hat{\mathcal{W}}[t_i, t_{i+1}]\{-z_{i,t_i} + z_{i+1,t_i}\} \\ &= \mathcal{M}_i\left[z_{i,t_i}\mathcal{W}[t_i, t_{i+1}]\right] - z_{i+1,t_i}\mathcal{M}_i\left[\mathcal{W}[t_i, t_{i+1}]\right], \end{aligned} \tag{I.8}$$

that brings the desired expression (I.4). The same procedure can be used to demonstrate that

$$\mathcal{M}_i\left[z^*_{i,t_i}\mathcal{W}[t_i, t_{i+1}]\right] = \int_{t_{i+1}}^{t_i} d\tau \mathcal{M}_i\left[z^*_{i,t_i} z_{i,\tau}\right]\mathcal{M}_i\left[\left(\frac{\delta\mathcal{W}[t_i, t_{i+1}]}{\delta z_{i,\tau}}\right)\right]. \tag{I.9}$$

Appendix J
Novikov property up to second order in perturbation parameter

There is an alternative possibility to the Novikov theorem (5.79), which consists in replacing the reduced propagators by their first order expansion

$$
\begin{aligned}
G(z_1^* z_0|t0) &= \left(1+\int_0^t d\tau z_{1,\tau}^* V_{\tau-t} L - \int_0^t d\tau z_{0\tau} V_{\tau-t} L^\dagger\right) G^{(}0)(z_1^* 0 z_0|t0);\\
G^\dagger(z_0^* z_1|0t) &= G^{\dagger,(0)}(z_0^* 0 z_1|0t)\left(1-\int_0^t d\tau z_{0,\tau}^* V_{\tau-t} L + \int_0^t d\tau z_{1,\tau} V_{\tau-t} L^\dagger\right) + \mathcal{O}(g^2),
\end{aligned}
\tag{J.1}
$$

where $G^{(}0)(z_1^* 0 z_0|t0) = \exp(-iH_S t)\exp(z_1^* z_0)$, and $G^{\dagger,(0)}(z_0^* 0 z_1|0t) = \exp(iH_S t)\exp(z_0^* z_1)$, and then performing the Gaussian integrals over the variables z_1. For instance, let us show that with the term

$$
\mathcal{M}_1\left[z_{1,t} G(z_1^* z_0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^* z_1|t0)L^\dagger\right]
\tag{J.2}
$$

on equation (5.77). Replacing (J.1) in the last expression, we get

$$
\begin{aligned}
&\mathcal{M}_1\left[z_{1,t} G(z_1^* z_0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^* z_1|t0)L^\dagger\right]\\
= &\int d\mu(z_1) z_{1,t} L \left(1+\int_0^t d\tau z_{1,\tau}^* V_{\tau-t} L - \int_0^t d\tau z_{0\tau} V_{\tau-t} L^\dagger\right) e^{-iH_S t} e^{z_1^* z_0}|\psi_0\rangle\\
&\langle\psi_0| e^{z_0^* z_1}\left(1-\int_0^t d\tau z_{0,\tau}^* V_{\tau-t} L + \int_0^t d\tau z_{1,\tau} V_{\tau-t} L^\dagger\right) e^{iH_S t} e^{z_0^* z_1} + \mathcal{O}(g^2).
\end{aligned}
\tag{J.3}
$$

In order to perform the average over z_1 it is necessary to take into account that $z_{1,t} = i\sum_{\lambda=1}^{\nu} g_\lambda z_{1,\lambda}\exp\left(-i\omega_\lambda t\right)$, so that the average $\mathcal{M}_1$ in fact represents a set of multi-dimensional integrals over each harmonic oscillator. For instance,

$$\begin{aligned}\mathcal{M}_1\left[z_{1,t}e^{z_1^* z_0}e^{z_0^* z_1}\right] &= i\sum_{\lambda=1}^{\nu} g_\lambda e^{-i\omega_\lambda t}\left(\int d\mu(z_{1,1})e^{z_{1,1}^* z_{0,1}}e^{z_{0,1}^* z_{1,1}}\dots\right.\\ &\left.\int d\mu(z_\lambda)z_{1,\lambda}e^{z_{1,\lambda}^* z_{0,\lambda}}e^{z_{0,\lambda}^* z_{1,\lambda}}\dots\int d\mu(z_{1,\nu})e^{z_{1,\nu}^* z_{0,\nu}}e^{z_{0,\nu}^* z_{1,\nu}}\right). \qquad (J.4)\end{aligned}$$

Taking into account this, and the following results for Gaussian integrals,

$$\begin{aligned}&\int d\mu(z_{1,\lambda})z_{1,\lambda}e^{z_{1,\lambda}^* z_{0,\lambda}}e^{z_{0,\lambda}^* z_{1,\lambda}} = z_{0,\lambda}e^{z_{0,\lambda}^* z_{0,\lambda}},\\ &\int d\mu(z_{1,\lambda}^*)z_{1,\lambda}^*e^{z_{1,\lambda}^* z_{0,\lambda}}e^{z_{0,\lambda}^* z_{1,\lambda}} = z_{0,\lambda}^*e^{z_{0,\lambda}^* z_{0,\lambda}},\\ &\int d\mu(z_{1,\lambda}^*)z_{1,\lambda}^* z_{1,\lambda}e^{z_{1,\lambda}^* z_{0,\lambda}}e^{z_{0,\lambda}^* z_{1,\lambda}} = (1+z_{0,\lambda}^* z_{0,\lambda})e^{z_{0,\lambda}^* z_{0,\lambda}}, \qquad (J.5)\end{aligned}$$

we get for (J.3),

$$\begin{aligned}&\mathcal{M}_1\left[z_{1,t}G(z_1^* z_0|t0)|\psi_0\rangle\langle\psi_0|G^\dagger(z_0^* z_1|t0)L^\dagger\right]\\ = \;& Lz_{0,t}\rho_s^{(1)}(z_0^* z_0|t) + L\int_0^t d\tau\alpha(t-\tau)V_{\tau-t}L\rho_s^{(0)}(z_0^* z_0|t). \qquad (J.6)\end{aligned}$$

In the former expression, we have specified explicitly the perturbative order of the density operator in each term, where

$$\begin{aligned}\rho_s^{(1)}(z_0^* z_0|t) &= e^{z_{0,\lambda}^* z_{0,\lambda}}\left(e^{-iH_S t}|\psi_0\rangle\langle\psi_0|e^{iH_S t} + \int_0^t d\tau z_{0,\tau}^*[V_{\tau-t}L, e^{-iH_S t}|\psi_0\rangle\langle\psi_0|e^{iH_S t}]\right.\\ &+ \left.\int_0^t d\tau z_{0,\tau}[e^{-iH_S t}|\psi_0\rangle\langle\psi_0|e^{iH_S t}, V_{\tau-t}L^\dagger]\right), \qquad (J.7)\end{aligned}$$

is the first order expansion, and $\rho_s^{(0)}(z_0^* z_0|t) = e^{-iH_S t}|\psi_0\rangle\langle\psi_0|e^{iH_S t}\exp\left(z_{0,\lambda}^* z_{0,\lambda}\right)$ is the zero order. This is done in order to make it easier for the reader to identifiy the terms with the results of the averages appearing in (J.3). However, since the whole expression (J.6) is of order g^2, we shall simplify the notation by just writing $\rho_s(z_0^* z_0|t)$ in every term. Evidently, it shall be understood that the equation is valid up to second order. The average of the term $z_{1,t}^*$ of (5.77) is made in an analogous way.

Appendix K
Derivation of the relation (8.15)

The functional derivative can be expressed in a more convenient way as follows. Let us take the equation (2.36)

$$\begin{aligned}\frac{\partial G(z_i^* z_{i+1}|t_i t_{i+1})}{\partial t_i} = & \left(- iH_S - iL\sum_\lambda g_\lambda e^{i\omega_\lambda t_i} z^*_{i,\lambda}\right) G(z_i^* z_{i+1}|t_i t_{i+1}) \\ & -iL^\dagger \sum_\lambda g_\lambda e^{-i\omega_\lambda t_i} \langle z_i | a_\lambda \mathcal{U}_I(t_i, t_{i+1}) | z_{i+1}\rangle, \end{aligned} \tag{K.1}$$

considering now that the term $\langle z_i | a_\lambda \mathcal{U}_I(t_i, t_{i+1}) | z_{i+1}\rangle$ can also be expressed as $\frac{\partial}{\partial z^*_{i,\lambda}} \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) | z_{i+1}\rangle = \frac{\partial}{\partial z^*_{i,\lambda}} G(z_i^* z_{i+1}|t_i t_{i+1})$. Considering again the separation (I.3) of the propagator, we can perform the partial derivative over the coordinate $z^*_{i,\lambda}$ as follows,

$$\begin{aligned}\frac{\partial}{\partial z^*_{i,\lambda}} G(z_i^* z_{i+1}|t_i t_{i+1}) = & \left(\frac{\partial G(z_i^* z_{i+1}|t_{i+1} t_{i+1})}{\partial z^*_{i,\lambda}} \right) \hat{G}(z_i^* z_{i+1}|t_i t_{i+1}) \\ & + G(z_i^* z_{i+1}|t_{i+1} t_{i+1}) \left(\frac{\partial \hat{G}(z_i^* z_{i+1}|t_i t_{i+1})}{\partial z^*_{i,\lambda}} \right). \end{aligned} \tag{K.2}$$

The first derivative appearing in the last expression is equal to $z_{i+1,\lambda}$, while the second can be solved using the chain rule,

$$\frac{\partial \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\partial z^*_{i,\lambda}} = \sum_\beta \frac{\partial \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\partial z^*_{i,t_{i,\beta}}} \frac{\partial z^*_{i,t_{i,\beta}}}{\partial z^*_{i,\lambda}}$$

$$
\begin{aligned}
&= \lim_{\epsilon\longrightarrow 0} \epsilon \left(\frac{1}{\epsilon} \frac{\partial \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\partial z^*_{i,t_{i,\beta}}} \right) \frac{\partial z^*_{i,t_{i,\beta}}}{\partial z^*_{i,\lambda}} \\
&= \int_{t_{i+1}}^{t_i} d\tau \frac{\delta \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\delta z^*_{i,\tau}} (-ig_\lambda e^{i\omega_\lambda \tau}), \qquad \text{(K.3)}
\end{aligned}
$$

where we have discretized the time t_i in intervals ϵ, in such a way that $t_{i,\beta} = \epsilon + t_{i,\beta-1} = t_0 + (\beta - 1)\epsilon$. Thus, the function z_{i,t_i} is approximated by a vector of values $z_{i,t_{i,\beta}} = \{\cdots z_{i,t_{i,\beta-1}}, z_{i,t_{i,\beta}} \cdots\}$. In the last line of (K.3), we have solved the partial derivative of $z^*_{i,t_{i,\beta}}$ using (7.47), and we have passed to the continuum limit, $\epsilon \rightarrow 0$, considering that in such limit, $\frac{1}{\epsilon}\frac{\partial \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\partial z^*_{i,t_{i,\beta}}} \rightarrow \frac{\delta \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\delta z^*_{i,\tau}}$ [1]. Replacing this results in (K.2) we get the following expression for the partial derivative,

$$
\frac{\partial}{\partial z^*_{i,\lambda}} G(z_i^* z_{i+1}|t_i t_{i+1}) = z_{i+1,\lambda} G(z_i^* z_{i+1}|t_i t_{i+1}) - ig_\lambda \int_{t_{i+1}}^{t_i} d\tau \frac{\delta G(z_i^* z_{i+1}|t_i t_{i+1})}{\delta z^*_{i,\tau}} e^{i\omega_\lambda \tau}. \qquad \text{(K.4)}
$$

Since

$$
\frac{\partial}{\partial z^*_{i,\lambda}} G(z_i^* z_{i+1}|t_i t_{i+1}) = \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) a_\lambda(t_i, t_{i+1}) | z_{i+1} \rangle \qquad \text{(K.5)}
$$

we can compare equation (K.4) with the expression that is obtained by replacing the analytical solution of $a_\lambda(t_i, t_{i+1})$ (2.38) in the right hand side of (K.5). Thus, it is found that

$$
\begin{aligned}
\frac{\partial}{\partial z^*_{i,\lambda}} G(z_i^* z_{i+1}|t_i t_{i+1}) &= \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) a_\lambda(t_i, t_{i+1}) | z_{i+1} \rangle = \\
&= z_{i+1,\lambda} G(z_i^* z_{i+1}|t_i t_{i+1}) - ig_\lambda \int_{t_{i-1}}^{t_i} d\tau \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle e^{i\omega_\lambda \tau}.
\end{aligned}
\qquad \text{(K.6)}
$$

Thus, we conclude that the functional derivative can be expressed as

$$
\frac{\delta G(z_i^* z_{i+1}|t_i t_{i+1})}{\delta z^*_{i,\tau}} = \langle z_i | \mathcal{U}_I(t_i, t_{i+1}) L(\tau, t_{i+1}) | z_{i+1} \rangle, \qquad \text{(K.7)}
$$

which is the relation (8.15).

---

[1] The functional derivative $\frac{\delta \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\delta z^*_{i,\tau}}$, is respect to continuous variables, in this case $\delta z^*_{i,\tau}$. The partial derivative $\frac{\partial \hat{G}(z_i^* z_{i+1}|t_{i,\beta} t_{i+1})}{\partial z^*_{i,t_{i,\beta}}}$ is respect to discrete variables, in this case $z^*_{i,t_{i,\beta}}$.

Appendix L
Thermal MTCF

As described in Section (2.2) of Chapter (2), MTCF can also be computed for initial states in which the environment is different from the vacuum. Suppose that we have an initially decorrelated state and a thermal mixture for the environment. Then, according to (2.19), we have

$$\rho_{tot}(0) = |\psi_0\rangle\langle\psi_0| \otimes \int d^2z_0 P(z_0, z_0^*)|z_0\rangle\langle z_0|, \tag{L.1}$$

where $P(z_0, z_0^*)$ is the coherent state P distribution [43, 53], which is this case is chosen as the one corresponding to a thermal reservoir (eqn. (5.84)) of Chapter (5),

$$P(z_0, z_0^*) = \prod_\lambda \frac{1}{\pi N(\omega_\lambda)} e^{-|z_0|^2 N(\omega_\lambda)}. \tag{L.2}$$

According to (2.20), the MTCF for such an initial state is

$$C^T_{\mathbf{A}}(\mathbf{t}|\rho_{tot}(0)) = \int d^2z_0 P(z_0, z_0^*) e^{-|z_0|^2} \langle\psi_0|\langle z_0|A_1(t_1)\cdots A_N(t_N)\rangle|z_0\rangle|\psi_0\rangle, \tag{L.3}$$

where the superindex T denotes the fact that it is a thermal MTCF. To compute the evolution equation of $C^T_{\mathbf{A}}(\mathbf{t}|\rho_{tot}(0))$, we consider the general equation (8.37) obtained in Section (8.3),

$$\begin{aligned} \frac{d\mathbf{A}(\mathbf{t})}{dt_1} &= i[H_S(t_1), A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \\ -& \quad \nu^\dagger(t_1)[L(t_1), A(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) + [L^\dagger(t_1), A(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})\nu(t_1) \\ +& \quad \int_0^{t_1} d\tau \alpha^*(t_1-\tau)L^\dagger(\tau)[A_1(t_1), L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \end{aligned}$$

$$
+ \sum_{i=0}^{N-1} \int_{t_{i+2}}^{t_{i+1}} d\tau \alpha(t_1 - \tau)[L^\dagger(t_1), A_1(t_1)]\mathcal{P}_L^i L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}). \tag{L.4}
$$

Then, from (L.3), we have that

$$
\begin{aligned}
&\frac{dC^T_{\mathbf{A}}(\mathbf{t}|\rho_{tot}(0))}{dt_1} = \int d^2 z_0 P(z_0, z_0^*) e^{-|z_0|^2} \\
&\langle\psi_0|\langle z_0| \Big(i[H_S(t_1), A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \\
- \;& \nu^\dagger(t_1)[L(t_1), A(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) + [L^\dagger(t_1), A(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})\nu(t_1) \\
+ \;& \int_0^{t_1} d\tau \alpha^*(t_1 - \tau) L^\dagger(\tau)[A_1(t_1), L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \\
+ \;& \sum_{i=0}^{N-1} \int_{t_{i+2}}^{t_{i+1}} d\tau \alpha(t_1 - \tau)[L^\dagger(t_1), A_1(t_1)]\mathcal{P}_L^i L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \Big) |z_0\rangle|\psi_0\rangle.
\end{aligned} \tag{L.5}
$$

In order to simplify the the calculus, let us particularize for two-time correlations,

$$
\begin{aligned}
&\frac{dC^T_{AB}(\mathbf{t}|\rho_{tot}(0))}{dt_1} = \frac{d\langle A(t_1)B(t_2)\rangle^T}{dt_1} = i\langle\{[H_S, A]\}(t_1)B(t_2)\rangle^T \\
+ \;& \int_0^{t_1} d\tau \alpha^*(t - \tau)\langle\left\{V_{\tau - t_1} L^\dagger [A, L]\right\}(t_1)B(t_2)\rangle^T \\
+ \;& \int_{t_2}^{t_1} d\tau \alpha(t - \tau)\langle\left\{[L^\dagger, A] V_{\tau - t_1} L\right\}(t_1)B(t_2)\rangle^T \\
+ \;& \int_0^{t_2} d\tau \alpha(t - \tau)\langle\left\{[L^\dagger, A]\right\}(t_1)\left\{B V_{\tau - t_2}\right\}(t_2)\rangle^T \\
+ \;& \int d^2 z_0 P(z_0, z_0^*) e^{-|z_0|^2} z_{0,t_1} \langle\psi_0|\langle z_0|[L^\dagger(t_1), A(t_1)]B(t_2)|z_0\rangle|\psi_0\rangle \\
+ \;& \int d^2 z_0 P(z_0, z_0^*) e^{-|z_0|^2} z^*_{0,t_1} \langle\psi_0|\langle z_0|[A(t_1), L(t_1)]B(t_2)|z_0\rangle|\psi_0\rangle.
\end{aligned} \tag{L.6}
$$

However, the procedure followed here is valid for general N-time correlations. In order to perform the average over the last two terms we follow a procedure similar to that explained in Section (5.2.1.2), to compute the thermal master equation. First of all, we express them in terms of reduced propagators by inserting the Bargmann closure relation twice. Second, we insert a perturbative expansion of the reduced propagators up to first order in g, since the noise is already of first order. Third, we compute the Gaussian integrals. The average over the term in z_{0,t_1} is then

$$
\begin{aligned}
&\int d^2 z_0 P(z_0, z_0^*) e^{-|z_0|^2} z_{0,t_1} \langle\psi_0|\langle z_0|\{[L^\dagger, A]\}(t_1)B(t_2)|z_0\rangle|\psi_0\rangle \\
= \;& \int_0^{t_1} d\tau \alpha^{+*}(t_1 - \tau)\langle\left\{V_{\tau - t_1} L [A, L^\dagger]\right\}(t_1)B(t_2)\rangle^T \\
+ \;& \int_{t_2}^{t_1} d\tau \alpha^{+*}(t_1 - \tau)\langle\left\{[L^\dagger, A] V_{\tau - t_1} L\right\}(t_1)B(t_2)\rangle^T \\
+ \;& \int_0^{t_2} d\tau \alpha^{+*}(t_1 - \tau)\langle\left\{[L^\dagger, A]\right\}(t_1)\left\{B V_{\tau - t_2} L\right\}(t_2)\rangle^T,
\end{aligned} \tag{L.7}
$$

and the average over the term in z^*_{0,t_1} is

$$\begin{aligned}
&\int d^2z_0 P(z_0,z_0^*)e^{-|z_0|^2} z^*_{0,t_1}\langle\psi_0|\langle z_0|[A(t_1),L(t_1)]B(t_2)|z_0\rangle|\psi_0\rangle \\
= &\int_0^{t_1} d\tau\alpha^+(t_1-\tau)\langle\left\{V_{\tau-t_1}L^\dagger[A,L]\right\}(t_1)B(t_2)\rangle^T \\
+ &\int_{t_2}^{t_1} d\tau\alpha^+(t_1-\tau)\langle\left\{[L,A]V_{\tau-t_1}L^\dagger\right\}(t_1)B(t_2)\rangle^T \\
&\int_0^{t_2} d\tau\alpha^+(t_1-\tau)\langle\{[L,A]\}(t_1)\left\{BV_{\tau-t_2}L^\dagger\right\}(t_2)\rangle^T,
\end{aligned} \tag{L.8}$$

where we consider the correlation defined as in (4.21),

$$\alpha^+(t-\tau) = \sum_\lambda g_\lambda^2 N(\omega_\lambda)e^{i\omega_\lambda(t-\tau)}. \tag{L.9}$$

Inserting (L.7) and (L.8) in (L.6), we get the evolution equation for thermal two-time correlation functions. As in Section(5.2.1.2) this equation can be simplified by considering a new correlation function which is defined as in (4.20),

$$\alpha^-(t-\tau) = \sum_\lambda g_\lambda^2(N(\omega_\lambda)+1)e^{-i\omega_\lambda(t-\tau)} = \alpha^{+*}(t-\tau)+\alpha(t-\tau). \tag{L.10}$$

In terms of $\alpha^+(t-\tau)$ and $\alpha^-(t-\tau)$, the thermal two-time correlations evolve as follows

$$\begin{aligned}
\frac{d\langle A(t_1)B(t_2)\rangle^T}{dt_1} = \; & i\langle\{[H_S,A]\}(t_1)B(t_2)\rangle^T + \\
+ &\int_0^{t_1} d\tau\alpha^{-*}(t-\tau)\langle\left\{V_{\tau-t_1}L^\dagger[A,L]\right\}(t_1)B(t_2)\rangle^T \\
+ &\int_{t_2}^{t_1} d\tau\alpha^-(t-\tau)\langle\left\{[L^\dagger,A]V_{\tau-t_1}L\right\}(t_1)B(t_2)\rangle^T \\
+ &\int_0^{t_2} d\tau\alpha^-(t-\tau)\langle\left\{[L^\dagger,A]\right\}(t_1)\left\{BV_{\tau-t_2}\right\}(t_2)\rangle^T \\
+ &\int_0^{t_1} d\tau\alpha^{+*}(t_1-\tau)\langle\left\{V_{\tau-t_1}L[A,L^\dagger]\right\}(t_1)B(t_2)\rangle^T \\
+ &\int_{t_2}^{t_1} d\tau\alpha^+(t_1-\tau)\langle\left\{[L,A]V_{\tau-t_1}L^\dagger\right\}(t_1)B(t_2)\rangle^T \\
+ &\int_0^{t_2} d\tau\alpha^+(t_1-\tau)\langle\{[L,A]\}(t_1)\left\{BV_{\tau-t_2}L^\dagger\right\}(t_2)\rangle^T.
\end{aligned} \tag{L.11}$$

In the case $B=1$, the former equation becomes the thermal evolution equation for the expectation value of A. It is easy to verify that such an evolution coincides with the one given by the thermal master equation (5.88).

Note that when $L=L^\dagger$ the former equation becomes equal to (9.20) but with $\alpha(t-\tau)=\alpha_T(t-\tau)=\alpha^+(t-\tau)+\alpha^-(t-\tau)=\sum_\lambda g_\lambda^2\left[\coth\left(\frac{\omega_\lambda\beta}{2}\right)\cos\left(\omega_\lambda(t-\tau)\right)-i\sin\left(\omega_\lambda(t-\tau)\right)\right]$ given by (5.25).

Appendix M
Measurement-like MTCF

Multiple-time correlation functions may correspond to direct measurement when they have the following form [1]

$$C_{\mathbf{A}',\mathbf{A}}(\mathbf{t}',\mathbf{t}|\Psi_0) = \langle\Psi_0|A'_N(t'_N)\cdots A'_2(t'_2)A_1(t_1)\cdots A_N(t_N)|\Psi_0\rangle, \tag{M.1}$$

where the time ordering is such that

$$\begin{aligned} t'_N &\leq t'_{N-1} \leq \cdots \leq t'_2 \leq t_1 \\ t_N &\leq t_{N-1} \leq \cdots \leq t_2 \leq t_1. \end{aligned} \tag{M.2}$$

Let us show that by considering a sequence of measurements on a well defined initial quantum state of the system $|\Psi_0\rangle = |\psi_0\rangle|0\rangle$. The state vector of the system after having measured $q-1$ times with results $\tilde{a}_1, \tilde{a}_2, \cdots \tilde{a}_{q-1}$, the system state vector is

$$|\Psi_{\tilde{a}_1,\tilde{a}_2,\cdots\tilde{a}_{q-1}}(t_{q-1})\rangle \tag{M.3}$$

During the time between succesive measurements, the system will evolve unitarily as

$$|\Psi_{\tilde{a}_1,\tilde{a}_2,\cdots\tilde{a}_{q-1}}(t_q)\rangle = \mathcal{U}(t_q,t_{q-1})|\Psi_{\tilde{a}_1,\tilde{a}_2,\cdots\tilde{a}_{q-1}}(t_{q-1})\rangle \tag{M.4}$$

---

[1] The definition of the measurement-like form of correlation function presented in this section has been taken from the book [51], where it is also shown how its evolution equation for the Markovian case and in the weak coupling limit obeys the same structure as the Quantum Regression Theorem. The derivation of a non-Markovian evolution equation, both in its exact (open) form and in the weak coupling limit is a result of this thesis.

The measurements, performed at times $t_q, q = 1, 2, 3 \cdots,$, with $t_q > t_{q-1}$, are represented by the measuring operator $\tilde{\gamma}_{\tilde{a}_q}$, where $\tilde{a}_q$ is the result of the measurement. Thus, performing the measurement at time t_q over the former vector, we get

$$|\Psi_{\tilde{a}_1,\tilde{a}_2,\cdots\tilde{a}_q}(t_q)\rangle = \frac{\tilde{\gamma}_{\tilde{a}_q}|\Psi_{\tilde{a}_1,\tilde{a}_2,\cdots\tilde{a}_{q-1}}(t_q)\rangle}{\sqrt{P(\tilde{a}_q|\tilde{a}_1,\tilde{a}_2\cdots\tilde{a}_{q-1})}} = \frac{\prod_{r=1}^{q}\gamma_{\tilde{a}_r}\mathcal{U}(t_r,t_{r-1})|\Psi_0\rangle}{\sqrt{P(\tilde{a}_1,\cdots,\tilde{a}_q)}}, \tag{M.5}$$

where $P(\tilde{a}_1,\cdots,\tilde{a}_q) = \prod_{r=1}^{q} P(\tilde{a}_r|\tilde{a}_1,\cdots,\tilde{a}_{r-1})$ is the joint probability. This can be written as,

$$P(\tilde{a}_1,\cdots,\tilde{a}_q) = \langle\Psi_0|\left[\prod_{r=1}^{q}\tilde{\gamma}_{\tilde{a}_r}\mathcal{U}(t_r,t_{r-1})\right]^{\dagger}\prod_{r=1}^{q}\tilde{\gamma}_{\tilde{a}_r}\mathcal{U}(t_r,t_{r-1})|\Psi_0\rangle = \langle\Psi_0|\tilde{\gamma}^{\dagger}_{\tilde{a}_1}(t_1)\cdots\tilde{\gamma}^{\dagger}_{\tilde{a}_q}(t_q)\tilde{\gamma}_{\tilde{a}_q}(t_q)\cdots\tilde{\gamma}_{\tilde{a}_1}(t_1)|\Psi_0\rangle, \tag{M.6}$$

with $\tilde{\gamma}_{\tilde{a}_q}(t_q) = \mathcal{U}^{\dagger}(t_q,t_{q-1})\tilde{\gamma}_{\tilde{a}_q}\mathcal{U}(t_q,t_{q-1})$. The joint probability can also correspond to the multiple time correlation of any arbitrary operation $\theta(\tilde{a},t)$,

$$P(\tilde{a}_1,\cdots,\tilde{a}_q) = \langle\Psi_0|\theta^{\dagger}_{\tilde{a}_1}(t_1)\cdots\theta^{\dagger}_{\tilde{a}_q}(t_q)\theta_{\tilde{a}_q}(t_q)\cdots\theta_{\tilde{a}_1}(t_1)|\Psi_0\rangle. \tag{M.7}$$

Let us now recall the polarization identity,

$$A^{\dagger}MB = \frac{1}{4}\left\{(A+B)^{\dagger}M(A+B) - (A-B)^{\dagger}M(A-B) - i(A+iB)^{\dagger}M(A+iB) + i(A-iB)^{\dagger}M(A-iB)\right\} \tag{M.8}$$

which for $M = 1$ relates an arbitrary combination of operators in the left hand side, with a sum of different probabilities which as we have shown, can indeed be measured. Thus, any arbitrary correlation of the form (M.1) can be expressed as corresponding to a sum of measurable objects, provided that the time ordering is respected.

In order to obtain the evolution equation for these kind of measurement-like correlations, we use the Heisenberg method explained in section (8.2) of Chapter (9).

M.1 THREE TIME CORRELATION FUNCTION

We start by deriving the evolution equation of a measurement-like three time correlation function. In order to do that, let us consider the following equation,

$$\begin{aligned}\frac{dB'(t_2')A(t_1)B(t_2)}{dt_1} &= iB'(t_2')\mathcal{U}^{-1}(t_1)[H_{tot},A]\mathcal{U}(t_1)B(t_2) = \\ = \quad & iB'(t_2')[H_S(t_1),A(t_1)]B(t_2) + i\sum_{\lambda}g_{\lambda}\Big(B'(t_2')a^{\dagger}_{\lambda}(t_1)[L(t_1),A(t_1)]B(t_2) \\ + \quad & B'(t_2')[L^{\dagger}(t_1),A(t_1)]a_{\lambda}(t_1)B(t_2)\Big).\end{aligned} \tag{M.9}$$

This equation becomes a three-time correlation when making an average over the initial total state vector $|\Psi_0\rangle$. When $t_2' = t_2$ then it is a two-time correlation function. In order to eliminate the dependency on the environmental operator once the average over the total system initial state is performed, it is now necessary to make the following steps:

- Move the annihilation operator to the right hand side of the expression, considering once again expression (8.31)

$$\begin{aligned} & a_\lambda(t_1)B(t_2) = \mathcal{U}^{-1}(t_2)a_\lambda(t_1,t_2)B\mathcal{U}(t_2) \\ = \; & \mathcal{U}^{-1}(t_2)e^{-i\omega_\lambda(t_1-t_2)}a_\lambda(0)B\mathcal{U}(t_2) - ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2) \\ = \; & e^{-i\omega_\lambda t_1}B(t_2)a(0) - ig_\lambda\int_0^{t_2} d\tau e^{-i\omega_\lambda(t_1-\tau)}B(t)L(\tau) \\ - \; & ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2), \end{aligned} \tag{M.10}$$

  where we have used the solution (8.25) and

$$a_\lambda(t_1,t_2) = e^{-i\omega_\lambda(t_1-t_2)}a(0) - ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau,t_2), \tag{M.11}$$

  and the fact that $[B, a(0)] = 0$.

- Move the creation operator to the left hand side, so that following an analogous procedure we get

$$\begin{aligned} & B'(t'_2)a^\dagger_\lambda(t_1) = a^\dagger(0)B'(t'_2)e^{i\omega_\lambda t_1} + ig_\lambda\int_0^{t'_2} d\tau e^{i\omega_\lambda(t_1-\tau)}L^\dagger(\tau)B'(t'_2) \\ + \; & ig_\lambda\int_{t'_2}^{t_1} d\tau e^{i\omega_\lambda(t_1-\tau)}B'(t'_2)L^\dagger)(\tau). \end{aligned} \tag{M.12}$$

Replacing (M.10) and (M.12) in (M.9), we obtain the following

$$\begin{aligned} & \frac{dB'(t'_2)A(t_1)B(t_2)}{dt_1} = iB'(t'_2)[H_S(t_1),A(t_1)]B(t_2) - \nu^\dagger(t_1)B'(t'_2)[L(t_1),A(t_1)]B(t_2) \\ - \; & \int_0^{t'_2} d\tau\alpha^*(t_1-\tau)L^\dagger(\tau)B'(t'_2)[L(t_1),A(t_1)]B(t_2) \\ - \; & \int_{t'_2}^{t_1} d\tau\alpha(t_1-\tau)B'(t'_2)L^\dagger(\tau)[L(t_1),A(t_1)]B(t_2) \\ + \; & B'(t'_2)[L^\dagger(t_1),A(t_1)]B(t_2)\nu(t_1) + \int_0^{t_2} d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]B(t_2)L(\tau) \\ + \; & \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)[L^\dagger(t_1),A(t_1)]L(\tau)B(t_2) \end{aligned} \tag{M.13}$$

The evolution of the quantum mean value $\langle B'(t'_2)A(t_1)B(t_2)\rangle$ is again obtained by applying the total initial state on both sides of the former expression. When such initial state is $\mid \psi_0\rangle \mid 0\rangle$, the terms which depend on $\nu(t_1)$ and $\nu^\dagger(t_1)$ vanishes, and the final expression reads as follows,

$$\frac{d\langle\Psi_0|B'(t'_2)A(t_1)B(t_2)|\Psi_0\rangle}{dt_1} = i\langle\Psi_0|B'(t'_2)[H_S(t_1),A(t_1)]B(t_2)|\Psi_0\rangle$$

$$\begin{aligned}
&- \int_0^{t'_2} d\tau\alpha^*(t_1-\tau)\langle\Psi_0|L^\dagger(\tau)B'(t'_2)[L(t_1),A(t_1)]B(t_2)|\Psi_0\rangle \\
&- \int_{t'_2}^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0|B'(t'_2)L^\dagger(\tau)[L(t_1),A(t_1)]B(t_2)|\Psi_0\rangle \\
&+ \int_0^{t_2} d\tau\alpha(t_1-\tau)\langle\Psi_0|B'(t'_2)[L^\dagger(t_1),A(t_1)]B(t_2)L(\tau)|\Psi_0\rangle \\
&+ \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0|B'(t'_2)[L^\dagger(t_1),A(t_1)]L(\tau)B(t_2)|\Psi_0\rangle. \qquad \text{(M.14)}
\end{aligned}$$

M.2 FOUR-TIME CORRELATION FUNCTION

In order to derive the evolution equation of four measurement-like four-time correlations, we start from

$$\begin{aligned}
&\frac{dC'(t'_3)B'(t'_2)A(t_1)B(t_2)C(t_3)}{dt_1} = iC'(t'_3)B'(t'_2)\mathcal{U}^{-1}(t_1)[H_{tot},A]\mathcal{U}(t_1)B(t_2)C(t_3) \\
=\;& iC'(t'_3)B'(t'_2)[H_S(t_1),A(t_1)]B(t_2)C(t_3) \\
+\;& i\sum_\lambda g_\lambda\Big(C'(t'_3)B'(t'_2)a^\dagger_\lambda(t_1)[L(t_1),A(t_1)]B(t_2)C(t_3) \\
+\;& C'(t'_3)B'(t'_2)[L^\dagger(t_1),A(t_1)]a_\lambda(t_1)B(t_2)C(t_3)\Big). \qquad \text{(M.15)}
\end{aligned}$$

Again, we use the two-step method which consists in:

- Moving the annihilation operator $a_\lambda(t_1)$ to the right hand side of the equation (M.15). Carrying on operations analogous to those explained in the former section, we have

$$\begin{aligned}
&a_\lambda(t_1)B(t_2)C(t_3) = \mathcal{U}^{-1}(t_2)e^{-i\omega_\lambda(t_1-t_2)}a_\lambda(0)B\mathcal{U}(t_2)C(t_3) \\
-\;& ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2)C(t_3) \\
=\;& e^{-i\omega_\lambda(t_1-t_2)}B(t_2)\mathcal{U}^{-1}(t_3)a(t_2,t_3)C\mathcal{U}(t_3) - ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2)C(t_3) \\
=\;& B(t_2)C(t_3)a(0)e^{-i\omega_\lambda t_1} - ig_\lambda\int_{t_2}^{t_1} d\tau e^{-i\omega_\lambda(t_1-\tau)}L(\tau)B(t_2)C(t_3) \\
-\;& ig_\lambda\int_{t_3}^{t_2} d\tau)e^{-i\omega_\lambda(t_1-\tau)}B(t_2)L(\tau)C(t_3) \\
-\;& ig_\lambda\int_0^{t_3} d\tau)e^{-i\omega_\lambda(t_1-\tau)}B(t_2)C(t_3)L(\tau). \qquad \text{(M.16)}
\end{aligned}$$

- Moving the creation operator $a^\dagger_\lambda(t_1)$ to the left hand side of equation (M.15). After several operations of the usual type, one obtains

$$C'(t'_3)B'(t'_2)a^\dagger_\lambda(t_1) = a^\dagger(0)C'(t'_3)B'(t'_2)e^{i\omega_\lambda t_1}$$

$$
\begin{aligned}
&+ \quad iq_\lambda \int_{t'_2}^{t_1} d\tau e^{i\omega_\lambda(t_1-\tau)} C'(t'_3)B'(t'_2)L^\dagger(\tau) \\
&+ \quad ig_\lambda \int_{t'_3}^{t'_2} d\tau e^{i\omega_\lambda(t_1-\tau)} C'(t'_3)L^\dagger B'(t'_2) \\
&+ \quad ig_\lambda \int_{0}^{t'_3} d\tau e^{i\omega_\lambda(t_1-\tau)} L^\dagger(\tau)C'(t'_3)B'(t'_2).
\end{aligned}
\tag{M.17}
$$

Inserting the last expressions in (M.15), we get the following equation,

$$
\begin{aligned}
&\frac{dC'(t'_3)B'(t'_2)A(t_1)B(t_2)C(t_3)}{dt_1} = iC'(t'_3)B'(t'_2)[H_S(t_1), A(t_1)]B(t_2)C(t_3) \\
&- \quad \nu^\dagger(t_1)C'(t'_3)B'(t'_2)[L(t_1), A(t_1)]B(t_2)C(t_3) \\
&- \quad \int_{t'_2}^{t_1} d\tau\alpha^*(t_1-\tau)C'(t'_3)B'(t'_2)L^\dagger(\tau)[L(t_1), A(t_1)]B(t_2)C(t_3) \\
&- \quad \int_{t'_3}^{t'_2} d\tau\alpha^*(t_1-\tau)C'(t'_3)L^\dagger(\tau)B'(t'_2)[L(t_1), A(t_1)]B(t_2)C(t_2) \\
&- \quad \int_{0}^{t'_3} d\tau\alpha^*(t_1-\tau)L^\dagger(\tau)C'(t'_3)B'(t'_2)[L(t_1), A(t_1)]B(t_2)C(t_2) \\
&+ \quad C'(t'_3)B'(t'_2)[L^\dagger(t_1), A(t_1)]B(t_2)C(t_3)\nu(t_1) \\
&+ \quad \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)[L^\dagger(t_1), A(t_1)]L(\tau)B(t_2)C(t_3) \\
&+ \quad \int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)[L^\dagger(t_1), A(t_1)]B(t_2)L(\tau)C(t_3) \\
&+ \quad \int_{0}^{t_3} d\tau\alpha(t_1-\tau)[L^\dagger(t_1), A(t_1)]B(t_2)C(t_3)L(\tau)
\end{aligned}
\tag{M.18}
$$

Once the initial values for the total wave vector are applied on both sides, and provided that the bath initial state is $\mid 0\rangle$, the former equation has the following form

$$
\begin{aligned}
&\frac{d\langle\Psi_0|C'(t'_3)B'(t'_2)A(t_1)B(t_2)C(t_3)|\Psi_0\rangle}{dt_1} = \\
&= \quad i\langle\Psi_0|C'(t'_3)B'(t'_2)[H_S(t_1), A(t_1)]B(t_2)C(t_3)|\Psi_0\rangle \\
&- \quad \int_{t'_2}^{t_1} d\tau\alpha^*(t_1-\tau)\langle\Psi_0|C'(t'_3)B'(t'_2)L^\dagger(\tau)[L(t_1), A(t_1)]B(t_2)C(t_3)|\Psi_0\rangle \\
&- \quad \int_{t'_3}^{t'_2} d\tau\alpha^*(t_1-\tau)\langle\Psi_0|C'(t'_3)L^\dagger(\tau)B'(t'_2)[L(t_1), A(t_1)]B(t_2)C(t_3)|\Psi_0\rangle \\
&- \quad \int_{0}^{t'_3} d\tau\alpha^*(t_1-\tau)\langle\Psi_0|L^\dagger(\tau)C'(t'_3)B'(t'_2)[L(t_1), A(t_1)]B(t_2)C(t_3)|\Psi_0\rangle \\
&+ \quad \int_{t_2}^{t_1} d\tau\alpha(t_1-\tau)\langle\Psi_0|C'(t'_3)B'(t'_2)[L^\dagger(t_1), A(t_1)]L(\tau)B(t_2)C(t_3)|\Psi_0\rangle \\
&+ \quad \int_{t_3}^{t_2} d\tau\alpha(t_1-\tau)\Psi_0|C'(t'_3)B'(t'_2)[L^\dagger(t_1), A(t_1)]B(t_2)L(\tau)C(t_3)|\Psi_0\rangle
\end{aligned}
$$

$$+\quad\int_0^{t_3} d\tau\alpha(t_1-\tau)\Psi_0|C'(t'_3)B'(t'_2)[L^\dagger(t_1),A(t_1)]B(t_2)C(t_3)L(\tau)|\Psi_0\rangle \tag{M.19}$$

M.3 GENERALIZATION TO A $2N+1$-TIME CORRELATION FUNCTION

Let us now present the evolution equation for of a general measurement-like N-time correlation function defined in (M.1) as

$$C_{\mathbf{A}',\mathbf{A}}(\mathbf{t}',\mathbf{t}|\Psi_0)=\langle\Psi_0|A'_N(t'_N)\cdots A'_2(t'_2)A_1(t_1)\cdots A_N(t_N)|\Psi_0\rangle, \tag{M.20}$$

where the time ordering is such that

$$\begin{aligned} &t'_N\le t'_{N-1}\le\cdots\le t'_2\le t_1\\ &t_N\le t_{N-1}\le\cdots\le t_2\le t_1 \end{aligned} \tag{M.21}$$

In order to write the general equation, we use the superoperator $\mathcal{P}_R$, which translate $L(\tau)$ inside the string $\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})$ in the right direction according to (8.39), and define also an analogous superoperator $\mathcal{P}_R$ which acts over $\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})$ as follows

$$\begin{aligned} &\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})L^\dagger(\tau)\mathcal{P}_L^0=\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})L^\dagger(\tau)\\ &\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})L^\dagger(\tau)\mathcal{P}_L^1=\tilde{\mathbf{A}'}^{(\mathbf{3})}(\tilde{\mathbf{t}'}^{(\mathbf{3})})L^\dagger(\tau)A'_2(t'_2)\\ &\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})L^\dagger(\tau)\mathcal{P}_L^1=\tilde{\mathbf{A}'}^{(\mathbf{4})}(\tilde{\mathbf{t}'}^{(\mathbf{4})})L^\dagger(\tau)A'_3(t'_3)A'_2(t'_2)\\ \cdots\\ &\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})L^\dagger(\tau)\mathcal{P}_L^{N-1}=L^\dagger(\tau)\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})}). \end{aligned} \tag{M.22}$$

Here we have defined the string of operators $A'_N(t'_N)\cdots A'_2(t'_2)=\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})$, where $\tilde{\mathbf{t}'}^{(\mathbf{2})}=\{t'_N\cdots t'_2\}$, and in a similar way to (8.36) we set

$$\tilde{A'}^{(n)}(\tilde{\mathbf{t}'}^{(\mathbf{n})})=A'_N(t'_N)\cdots A'_n(t'_n), \tag{M.23}$$

with $\tilde{\mathbf{t}'}^{(\mathbf{n})}=\{t'_N\cdots t'_n\}$.

Within that notation, the evolution for 2N-time measurement-like correlation functions reads as follows

$$\begin{aligned} &\frac{dC_{\mathbf{A},\mathbf{A}'}(\mathbf{t},\mathbf{t}'|\Psi_0)}{d_t 1}=\langle\Psi_0\mid\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})[H_S(t_1),A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})\mid\Psi_0\rangle\\ +\quad&\sum_{i=0}^{N-1}\int_{t_{i+2}}^{t_{i+1}} d\tau\alpha^*(t_1-\tau)\langle\Psi_0\mid\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})L^\dagger(\tau)\mathcal{P}_L^i[A_1(t_1),L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})\mid\Psi_0\rangle\\ +\quad&\sum_{i=0}^{N-1}\int_{t_{i+2}}^{t_{i+1}} d\tau\alpha(t_1-\tau)\langle\Psi_0\mid\tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})[L^\dagger(t_1),A_1(t_1)]\\ &\times\mathcal{P}_R^i L(\tau)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})})\mid\Psi_0\rangle \end{aligned} \tag{M.24}$$

M.3.1 Generalization to a second order perturbative $2N+1$-time correlation function

In order to obtain a closed equation for measurement-like N-time correlation functions, it is often necessary to consider some approximation. Particularly, within the weak coupling limit, it is possible to obtain a general evolution equation up to second order in the perturbation parameter g. In that case, we use the superoperator $\mathcal{P}_R$ that acts over the string $\{V_{\tau-t_1}L\}(t_1)\{A_2(t_2)\cdots A_N(t_N)\}$ as described in (9.22),

$$\begin{aligned}
&\mathcal{P}_R^0\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) = \{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})})\\
&\mathcal{P}_R^1\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) = A_2(t_2)\{V_{\tau-t_2}L\}(t_2)\hat{\mathbf{A}}^{(\mathbf{3})}(\hat{\mathbf{t}}^{(\mathbf{3})}),\\
&\mathcal{P}_R^2\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) = A_2(t_2)A_3(t_3)\{V_{\tau-t_3}L\}(t_3)\hat{\mathbf{A}}^{(\mathbf{4})}(\hat{\mathbf{t}}^{(\mathbf{4})}),\\
\ldots&\\
&\mathcal{P}_R^{N-1}\{V_{\tau-t_1}L\}(t_1)\hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})}) = \hat{\mathbf{A}}^{(\mathbf{2})}(\hat{\mathbf{t}}^{(\mathbf{2})})\{V_{\tau-t_N}L\}(t_N),
\end{aligned} \tag{M.25}$$

and define a new superoperator $\mathcal{P}_L$ that acts over the string $\{V_{\tau-t_1}L\}(t_1)\{A_2(t_2)\cdots A_N(t_N)\}$ as,

$$\begin{aligned}
&\hat{\mathbf{A}'}^{(\mathbf{2})}(\hat{\mathbf{t}'}^{(\mathbf{2})})\{V_{\tau-t_1}L^\dagger\}(t_1)\mathcal{P}_L^0 = \hat{\mathbf{A}'}^{(\mathbf{2})}(\hat{\mathbf{t}'}^{(\mathbf{2})})\{V_{\tau-t_1}L^\dagger\}(t_1)\\
&\hat{\mathbf{A}'}^{(\mathbf{2})}(\hat{\mathbf{t}'}^{(\mathbf{2})})\{V_{\tau-t_1}L^\dagger\}(t_1)\mathcal{P}_L^1 = \hat{\mathbf{A}'}^{(\mathbf{3})}(\hat{\mathbf{t}'}^{(\mathbf{3})})\{V_{\tau-t'_2}L^\dagger\}(t'_2)A'_2(t'_2)\\
&\hat{\mathbf{A}'}^{(\mathbf{2})}(\hat{\mathbf{t}'}^{(\mathbf{2})})\{V_{\tau-t_1}L^\dagger\}(t_1)\mathcal{P}_L^2 = \hat{\mathbf{A}'}^{(\mathbf{4})}(\hat{\mathbf{t}'}^{(\mathbf{4})})\{V_{\tau-t'_3}L^\dagger\}(t'_3)A'_3(t'_3)A'_2(t'_2)\\
&\ldots\\
&\hat{\mathbf{A}'}^{(\mathbf{2})}(\hat{\mathbf{t}'}^{(\mathbf{2})})\{V_{\tau-t_1}L^\dagger\}(t_1)\mathcal{P}_L^{N-1} = \{V_{\tau-t'_N}L^\dagger\}(t'_N)\hat{\mathbf{A}'}^{(\mathbf{2})}(\hat{\mathbf{t}'}^{(\mathbf{2})})
\end{aligned} \tag{M.26}$$

Thus, the perturbative $2N-1$-time correlation reads as follows,

$$\begin{aligned}
&\frac{dC_{\mathbf{A}}(\mathbf{t}|\Psi_0)}{d_t1} = \langle\Psi_0 \mid \tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})[H_S(t_1), A_1(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle\\
+\quad &\sum_{i=0}^{N-1}\int_{t_{i+2}}^{t_{i+1}} d\tau\alpha^*(t_1-\tau)\langle\Psi_0 \mid \tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(2)})\{V_{\tau-t_1}L^\dagger\}(t_1)\mathcal{P}_L^i[A_1(t_1), L(t_1)]\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle\\
+\quad &\sum_{i=0}^{N-1}\int_{t_{i+2}}^{t_{i+1}} d\tau\alpha(t_1-\tau)\langle\Psi_0 \mid \tilde{\mathbf{A}'}^{(\mathbf{2})}(\tilde{\mathbf{t}'}^{(\mathbf{2})})[L^\dagger(t_1), A_1(t_1)]\mathcal{P}_L^i\{V_{\tau-t_1}L\}(t_1)\tilde{\mathbf{A}}^{(\mathbf{2})}(\tilde{\mathbf{t}}^{(\mathbf{2})}) \mid \Psi_0\rangle.
\end{aligned} \tag{M.27}$$

Appendix N
Accuracy of the environmental correlation function at short time

In section (11.3), we have stressed the advantage of the new correlation function we introduce, namely a more accurate description of the short time behavior. This might help to give a better description of non-Markovian effects in the atomic dynamics within this range. We also note that the derivation of such correlation function does not rely on the the stationary phase approximation. In the integral (11.12), the reason why the prefactor $\frac{|\hat{e}_k\sigma(\mathbf{R})\cdot\hat{u}_d|^2}{w(\mathbf{k})}$ can be considered constant is that it changes very slowly with the wave vector $\mathbf{k}$, *no matter how large is* τ *in the phase* $i\omega(\mathbf{k})\tau$. This can be easily verified numerically by comparing the integral (11.12),

$$\alpha(\tau) = \gamma(\frac{a}{2\pi})\sum_\sigma \int_{1BZ} dk \frac{|\hat{e}_k\sigma(R)\cdot\hat{u}_d|^2}{w(k)} e^{-i\omega(k)\tau}, \tag{N.1}$$

with

$$\alpha(\tau) = \sum_\sigma \frac{|\hat{e}_{k_0}\sigma(R)\cdot\hat{u}_d|^2}{w(k_0)} \gamma(\frac{a}{2\pi}) \int_{1BZ} dk e^{-i\omega(k)\tau}, \tag{N.2}$$

for the one-dimensional case, in which $\omega(k) = A + B\cos(ka)$. Here k_0 is a constant that has been chosen in such a way that both correlation functions are equal at $\tau = 0$

$$\int_{-\pi/a}^{\pi/a} dk \frac{1}{\omega(k)} = \frac{1}{\omega(k_0)} \int_{-\pi/a}^{\pi/a} dk \tag{N.3}$$

The factor $|\hat{e}_k \sigma(\mathbf{R}) \cdot \hat{u}_d|^2$ has been considered a constant, since it corresponds to a number from zero to one that does not affect the result dramatically (see Fig. (N.1)).

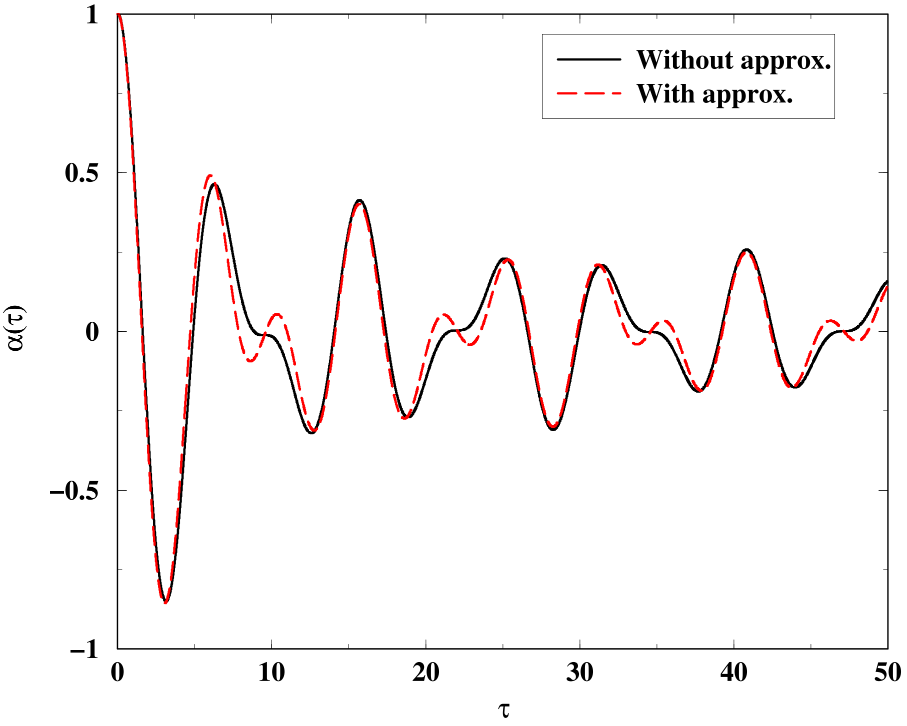

Fig. N.1 We compare numerically the integral (N.1) (solid line) with (N.2) (dashed line). Apart from some small deviations, it is shown that the approximation (N.2) is an accurate one even at short times.

Concerning the dispersion relation, a rigorous derivation or the model we propose is out of the scope of the thesis. However, we have introduced in the text some references about methods to derive dispersion relation for radiation field within PBG structures. Most of these methods are similar to those used for studying the band structure for electrons in solids, a fact that we believe justifies the use of a tight-binding approximation in our model. Although this model is rather simple and has been obtained for a simple cubic lattice, it contains all the essential features of the EM field in a photonic band gap material (see [120] for an example of band structure corresponding to the parameters used in the thesis). As a simple model, it might not be accurate enough to compute very precise quantities or the dynamic of systems within other photonic crystal structures. Although it would then be necessary to have more accurate dispersion relations, this would not change the methodology we have developed to obtain the correlation function, the corresponding noise, and to compute the dynamical equations.

Concerning the physical consequences of the dispersion relation we propose, it describes correctly the fluctuations of the EM field, which in our formalism are described by the quantity z_t. This description is not possible with a parabolic dispersion relation, since such a dispersion relation does not describe correctly the behavior in the center of the band. In addition, the dispersion relations that has been obtained both experimentally [120] and theoretically [118], are periodic functions, and not parabolic functions.

Appendix O
Photonic density of states (DOS) in the vacuum and in a PBG

As discussed in Chapter (1), the photonic DOS of a radiation field placed

$$\sum_{\mathbf{k}} \to \int d\omega D(\omega). \tag{O.1}$$

When the dispersion relation of the radiation field only depends on the modulus of the wave vector, the former integral in $\mathbf{k}$ can be solved in spherical coordinates,

$$\int_0^{2\pi} d\psi \int_0^{\pi} d\theta \sin\theta \left(\frac{2\upsilon}{(2\pi)^3} \right) \int_0^{\infty} dkd^2 = \int d\omega D(\omega). \tag{O.2}$$

This is the case of the vacuum, where the dispersion relation $\omega = ck$, so that $dk = d\omega/c$. Replacing in the last integral, we have

$$D(\omega) = \frac{\omega^2 \upsilon}{c^3 2\pi^2}. \tag{O.3}$$

In an anisotropic PC, the dispersion relation is the same as for a one dimensional PBG, namely $\omega = A + B\cos(ka)$ (see Section (11.3.2) for a derivation), so that

$$k = \frac{1}{a} arcos(\frac{\omega - A}{B}). \tag{O.4}$$

Then to transform the integral in k to an integral in ω, we need the following

$$dk = \left| \frac{-1}{aB\sqrt{s - \left(\frac{\omega - A}{B}\right)^2}} \right| d\omega, \tag{O.5}$$

which replaced in (O.2) together with (O.4) gives rise to the following photonic DOS

$$D(\omega) = \frac{1}{\pi^2} \frac{1}{aB\sqrt{s - \left(\frac{\omega - A}{B}\right)^2}} arcos(\frac{\omega - A}{B}). \tag{O.6}$$

Figure (O.1) represents the former expression compared to (O.3) (where we have chosen $c = 1$ and $\upsilon = 1$).

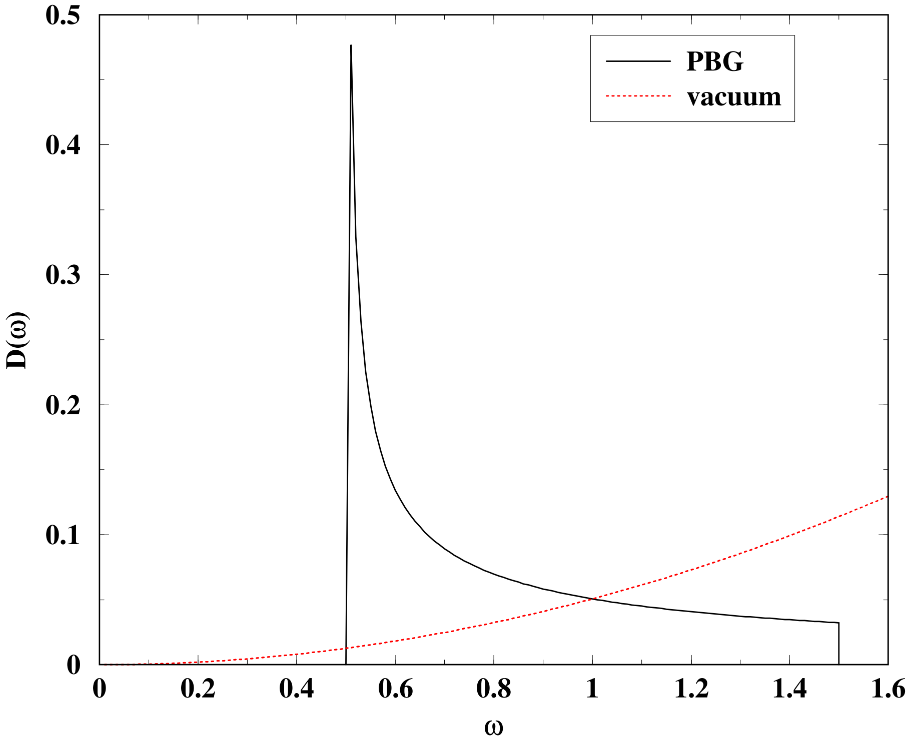

Fig. O.1 Photonic DOS of an anisotropic PC (O.6), compared to that of the vacuum (O.3). It is clearly observed how the last one only takes non-zero values within the band, which goes from $\omega_c = A - B$ to $\omega_c' = A + B$.

Appendix P
Numerical synthesis of the driving noise

There are several numerical methods in literature to generate a complex coloured Gaussian noise characterized by,

$$\begin{aligned}\mathcal{M}[z_t] = 0, \mathcal{M}[z_t z_\tau] = 0 \\ \mathcal{M}[z_t z_\tau^*] = \alpha(t-\tau),\end{aligned} \tag{P.1}$$

In particular, it can be synthesized [35] with the help of two independent real Gaussian noises ξ' and ξ'' such that

$$z_t = \int_{-\infty}^{\infty} d\tau R(\tau) \frac{\xi'(t-\tau) + i\xi''(t-\tau)}{\sqrt{2}}, \tag{P.2}$$

satisfying the properties

$$\begin{aligned}\mathcal{M}[\xi'(t)] = \mathcal{M}[\xi'(t)] = 0, \mathcal{M}[\xi'(t)\xi''(0)] = 0 \\ \mathcal{M}[\xi'(t)\xi'(0)] = \mathcal{M}[\xi''(t)\xi''(0)] = \delta(t).\end{aligned} \tag{P.3}$$

The function $R(\tau)$ that appears in the integral is known as the response function of the bath, and can be defined in terms of the correlation function as

$$\alpha(t) = \int_{-\infty}^{\infty} d\tau R^*(t+\tau) R(\tau). \tag{P.4}$$

In accordance with the former relation, the response function can be numerically calculated by performing the inverse Fourier transform of the power spectrum of the noise $\mathcal{G}(\omega)$,

$$R(t) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \mathcal{G}(\omega) e^{i\omega t}. \tag{P.5}$$

with,

$$|\mathcal{G}(\omega)|^2 = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \alpha(t) e^{-i\omega t}. \tag{P.6}$$

When calculating the function $\mathcal{G}(\omega)$ from (P.6), a complex phase θ appears, since $G\omega) = \sqrt{|\mathcal{G}(\omega)|^2} e^{i\theta}$. For simplicity, such phase can be chosen equal to zero.

Appendix Q
Density matrix in Pauli representation

In the Pauli representation, the density matrix becomes,

$$\rho = \frac{1}{2} Tr\rho \cdot I + \mathbf{a} \cdot \sigma, \tag{Q.1}$$

with $\mathbf{a} = (a_x, a_y, a_z)$ and $a_i = \frac{1}{2} Tr(\rho\sigma_i);\ i = x, y, z$. The matrices $\sigma_{x,y,z}$ are the usual Pauli matrices and $Tr\rho = 1$. In terms of $\langle\sigma_{ij}\rangle, i = 1, 2; j = 1, 2$, $a_x = 2\Re\langle\sigma_{12}\rangle$, $a_y = 2\Im\langle\sigma_{12}\rangle$ and $a_z = -\sigma_3$. From this relations and equation (Q.1), we finally obtain,

$$\begin{aligned}
\rho_{11}(t) &= \frac{1}{2} + a_z = \frac{1}{2} + \frac{\langle\sigma_{11}\rangle - \langle\sigma_{22}\rangle}{2} \\
\rho_{22}(t) &= \frac{1}{2} - a_z = \frac{1}{2} - \frac{\langle\sigma_{11}\rangle - \langle\sigma_{22}\rangle}{2} \\
\rho_{12}(t) &= a_x - ia_y = \langle\sigma_{21}\rangle \\
\rho_{21}(t) &= a_x + ia_y = \langle\sigma_{12}\rangle.
\end{aligned} \tag{Q.2}$$

Therefore, $\rho_3 = \rho_{22} - \rho_{11} = \sigma_{22} - \sigma_{11} = \sigma_3$.

18

Resumen de la tesis en español

18.1 INTRODUCCIÓN

En física, un sistema *aislado* es un objeto ideal, ya que procede de considerar como aproximación que sus interacciones con el medio son despreciables y no alteran significativamente la dinámica. No obstante, en muchas ocasiones, la interacción con el medio no sólo no se puede despreciar, sino que ademas es responsable de fenómenos físicos importantes. En tal caso, el sistema debe considerarse *abierto*.

Para describir la interacción, una posibilidad es integrar los grados de libertad del sistema total, compuesto por el sistema y su entorno[1]. No obstante, dado que el número de grados de libertad del entorno es por lo general muy grande, la integración de todos ellos puede llegar a ser una tarea muy pesada e incluso imposible. Sin embargo, no toda ésta información es necesaria para describir la dinámica del sistema abierto. En promedio, solo dos cantidades del medio actúan sobre dicha dinámica: sus fluctuaciones en el vacío, que pueden ser consideradas como un **ruido**, y la función de correlación de dichas fluctuaciones o **función de correlación del entorno**. El ruido describe el efecto aleatorio sobre el sistema de los múltiples grados de libertad del medio, mientras que la función de correlación describe la disipación o perdida de energía del sistema hacia dicho entorno. El tiempo de decaimiento de la función de correlación, también llamado *tiempo de memoria* es el empleado por el medio en recuperarse de la interacción con el sistema.

Un sistema abierto clásico se describe en términos de la densidad de probabilidad de sus coordenadas, o bien en término de dichas coordenadas. En el primer caso, la ecuación de movimiento es del tipo Chapman-Kolmogorov, que incorpora términos de tipo disipativo en los que interviene la función de correlación. La ecuación que rige la dinámica de las coordenadas del sistema es una ecuación del tipo Langevin, en la que aparte de los términos disipativos, intervienen términos de tipo estocástico en los que queda reflejada la acción aleatoria del baño. El promedio de las distintas trajectorias estocásticas generadas por la ecuación de Langevin da lugar a la función densidad de probabilidad obtenida por la ecuación de tipo Chapman-

---

[1] Habitualmente y para simplificar denominaremos "*sistema*" al sistema abierto, y "*sistema total*" o "*global*" al que está compuesto por el sistema abierto y su entorno.

Kolmogorov. Al añadir términos disipativos y fluctuantes, la dinámica ya no es reversible como lo es la dinámica de un sistema aislado.

El estudio de un sistema cuántico abierto supone adoptar un esquema de cuantización alternativo al del caso aislado, ya que este se basaba en la existencia de una función Lagrangiana o Hamiltoniana para el sistema. El esquema más comúnmente empleado consiste en suponer que el sistema total, compuesto por sistema y entorno, es conservativo y por tanto obedece las reglas de cuantización habituales. El estado de un sistema cuántico abierto no solo dependerá de los grados de libertad internos del mismo, sino también del estado en el que se encuentre el baño con el que interacciona. Se dice entonces que el estado cuántico del sistema está *enmarañado* con el entorno. En este ámbito, la fricción o disipación constituye una transferencia de energía desde el sistema 'pequeño' al entorno 'grande'. La energía, una vez transferida, se disipa en el entorno y no es devuelta al sistema en un tiempo físico relevante.

El estado de un sistema cuántico abierto es descrito por el operador densidad reducido del sistema, el cual se obtiene del operador densidad total a través de una traza parcial de los grados de libertad del entorno o baño, $\rho_s = Tr_B(\rho_{tot}(t))$. Este operador representa en general un estado mixto incluso aunque el estado total $\rho_{tot}(t)$, constituído por el sistema y el entorno, sea puro. El operador densidad fue introducido por Landau en el contexto de mecánica estadística [16], y por von-Neumann [15] para sistemas cuánticos fuera del equilibrio. La diagonal de este operador señala la probabilidad de cada estado del sistema cuántico en la base en la que el operador ha sido expresado. Por su parte, los elementos fuera de la diagonal señalan las coherencias, o interacciones entre los distintos estados del sistema. Las coherencias son propias de los sistemas cuánticos, y generalmente van desapareciendo a causa de la interacción, siguiendo un proceso que se conoce como decoherencia. Dicho proceso explica porqué los estados entrelazados característicos de un sistema cuántico no aparecen en el mundo macroscópico. El operador densidad reducido puede ser calculado a través de su ecuación dinámica, conocida como **ecuación maestra**, o realizando un promedio sobre los distintos estados de la mezcla estadística. Estos estados son soluciones de una **ecuación estocástica de Schrödinger (SSE)**.

Un ejemplo de sistema cuántico abierto encontrado en óptica cuántica es un átomo en contacto con el campo electromagnético circundante. La interacción, que da lugar a un intercambio de energía entre el átomo y el campo, produce en la mayor parte de los casos a una relajación del átomo a su estado fundamental, acompañada de una pérdida irreversible de su energía hacia el entorno. Cuando el operador densidad reducido está expresado en la base de estados propios del átomo, su diagonal indica la probabilidad de cada uno de los niveles de energía atómicos. Por su parte, los elementos fuera de la diagonal nos dan información acerca de las coherencias, que señalan en este caso la interación existente entre los distintos niveles de energía.

Si se promedia el estado del sistema total en los grados de libertad del baño, el *estado* resultante ya no evoluciona unitariamente, y dicha evolución deja de ser periódica, debido a la pérdida de energía o disipación que se produce en su interacción con el medio. Esto explica porque los sistemas cuánticos, que en estado de aislamiento son reversibles (en un tiempo de recurrecia finito vuelven a recuperar el estado inicial), presentan en la práctica una evolución disipativa y por tanto irreversible, al estar en la realidad sometidos a interacciones con el medio.

La dinámica de relajación atómica depende en gran parte de las fronteras y condiciones espaciales en las que está inmerso el campo electromagnético con el que interacciona. Este es un resultado conocido desde los trabajos de Purcell [10], más tarde ampliados por Kleppner [11], quienes observaron que el ritmo de relajación de un átomo de dos niveles emplazado en una cavidad puede ser aumentado con respecto a aquel del vacío cuando la longitud de ondas del fotón emitido es comparable a las dimensiones de la cavidad, e inhibida cuando no es así. La emisión puede ser modificada en gran medida también cuando el átomo es acoplado a un campo de radiación en un cristal en el que el índice de refracción es espacialmente periódico. Estos materiales, sugeridos inicialmente por Yablonovitch [12] y John [13], se conocen comúmente como **materiales de banda fotónica (MBF)** o **cristales fotónicos (CF)**.

En este punto surge la pregunta de cual es el mecanismo físico a través del cuál se modifica la dinámica del átomo cuando este está emplazado en un entorno estructurado. Dicha dinámica depende de la densidad de modos del campo entorno a la frecuencia de emisión, o **densidad fotónica de estados (DFE)**, y esta función es la que se modifica cuando el campo está immerso en un entorno estructurado, ya sea una cavidad cuántica, una guía de ondas, o un material de banda fotónica.

En el campo libre, la densidad fotónica de estados en una función que crece con ω^2, y que varía en un rango de frecuencias mayor que el ritmo de emisión espontánea. En estas condiciones, el fotón emitido es absorbido instantáneamente por el campo, lo que da lugar a un tiempo de memoria nulo. De este modo, la función de correlación que aparece en los términos disipativos de las ecuaciones dinámicas del átomo es una función delta, y el átomo decae exponencialmente hacia el estado fundamental, siguiendo un proceso descrito por la teoría de Wigner-Weisskopf [14]. Este tipo de interacción, que se conoce como **Markoviana**, puede también darse en una cavidad, pero, nuevamente, solo cuando la densidad de estados fotónica del campo, que en dicho entorno tiene la forma de una Lorentziana, varía suavemente en torno a la frecuencia de emisión del átomo. En las cavidades cuánticas, el ritmo de emisión espontánea aumenta cuando la frecuencia de emisión atómica se sitúa en la frecuencia del máximo de la Lorentziana o frecuencia de resonancia, y disminuye cuando se sitúa lejana a dicha frecuencia.

En algunos entornos estructurados, la densidad fotónica de estados presenta saltos discontinuos o comportamiento singular en un rango de frecuencias comparable con el ritmo de emisión espontánea. Esto ocurre por ejemplo en un CF. En éstos materiales, la periodicidad en el índice de refracción produce una reflexión de la luz hacia fuera del material para ciertas frecuencias que están relacionadas con dicha periodicidad. Dado que estos modos están ausentes del cristal, la densidad fotónica de estados es cero en las frecuencias correspondientes, por lo que se forma un *gap*. Los valores de frecuencia en los que la densidad fotónica de estados es no nula son conocidos como bandas. En los bordes de la banda, la densidad fotónica presenta una discontinuidad en la que pasa a tener un valor cero en el gap a tener un valor no nulo dentro de la banda. En dichas discontinuidades la velocidad de grupo de la luz tiende a cero, por lo que se produce una localización de los fotones. Cuando el átomo emite un fotón en dicha región, tiende a *congelarse* o localizarse en torno al mismo, lo que propicia que pueda ser reabsorbido por el átomo. El tiempo en el que el entorno se recupera de la interacción, o tiempo de memoria del campo, ya no es cero como en el caso Markoviano, sino que posee un valor finito que es característico de las interacciones **no-Markovianas**. En dichas interacciones, el decaimiento atómico ya no es exponencial, y puede además presentar oscilaciones debido al intercambio de energía entre los grados de libertad atómicos y fotónicos. Este tipo de comportamiento oscilatorio puede encontrarse también en una cavidad, cuando el rango de variación de la densidad fotónica de estados es comparable al ritmo de emisión espontánea.

En general, las ecuaciones maestras y las ecuaciones estocásticas de Schrödinger pueden ser tanto Markovianas como no-Markovianas, dependiendo de si la función de correlación que aparece en el término disipativo es una función delta o no, y, en el caso de EES, si el ruido es Gaussiano blanco o coloreado. No obstante, aunque el conocimiento del operador densidad reducido del sistema permite el cálculo de los valores medios de los operadores del sistema, la dinámica del mismo no se describe solo por tales cantidades. Para completar la descripción es preciso conocer las **funciones de correlación multitemporales (FCM)** de operadores del sistema. Por ejemplo, en óptica cuántica ciertas funciones de correlación a dos tiempos son necesarias para el cálculo del espectro de emisión de un átomo, o para describir la probabilidad condicionada de emisión de fotones.

Las funciones de correlación multitemporales son descritas en el caso Markoviano a través del denominado **teorema de regresión cuántico (TRC)**, que fue descubierto por Onsager (especialmente para el caso de fluctuaciones en torno al equilibrio) [17], y por Lax (para el caso más general de sistemas fuera del equilibrio) [18, 19]. Dicho teorema señala que la evolución de correlaciones a dos tiempos puede ser computada con una ecuación maestra para la matriz densidad reducida del sistema. Este resultado, puede generalizarse para funciones de correlación de N-tiempos, dado que éstas también obedecen la misma ecuación de evolución que los promedios cuánticos. El espectro atómico de emisión, que es la transformada de Fourier de una función de correlación a dos tiempos de los operadores de acoplamiento del sistema, es una Lorentziana, como corresponde a la transformada de Fourier de un decaimiento exponencial.

Para el caso no-Markoviano el espectro de emisión ya no es tan solo la transformada de Fourier de la función a dos tiempos de los operadores de acoplamiento, pero aún depende de tal correlación. No obstante, las funciones de correlación a dos tiempos, y en general las de N-tiempos, ya no pueden ser expresadas a través del teorema de regresión cuántico. Es preciso generar una teoría alternativa que describa funciones de correlación multitemporales no-Markovianas.

El objetivo de esta tesis es estudiar y desarrollar las ecuaciones dinámicas de un sistema cuántico abierto linearmente acoplado a un entorno de osciladores armónicos. Esto incluye las ecuaciones necesarias para evaluar sus valores medios, que son principalmente la ecuación maestra y la ecuación estocástica de Schrödinger, así como las ecuaciones que permiten el cómputo de funciones de correlación multitemporales. Todas ellas se derivan en particular para sistemas con interacción no-Markoviana, como es un átomo en contacto con el campo de radiación modificado en un cristal fotónico.

El trabajo se organiza en cuatro partes,

- En la Parte (I) se define el problema, presentando el tipo de sistemas estudiados, así como el objeto básico empleado para describir su dinámica. Esto se hace a lo largo de dos capítulos:
    - En el Capítulo (1), se presenta el modelo general de Hamiltoniano estudiado en esta tesis, cuyo término de interacción representa un acoplamiento lineal entre operadores del sistema y el entorno. En particular, se muestra cómo el Hamiltoniano de interacción de un átomo con el campo de radiación obedece a esta forma lineal cuando se aplican las aproximaciones dipolar y de onda rotante al modelo general de Hamiltoniano de un campo bosónico en contacto con un campo fermiónico.
    - En el Capítulo (2), derivamos el denominado **propagador reducido**, un objeto que evoluciona la función de ondas del sistema condicionada a un determinado estado inicial y final para el entorno, y obtenemos también su ecuación dinámica. El propagador reducido resulta ser la herramienta esencial para el cálculo de todas las ecuaciones dinámicas del sistema, ya sean valores medios cuánticos o funciones de correlación multitemporales.
- La Parte (II) se dedica al estudio de los valores medios cuánticos de sistemas abiertos no-Markovianos. Se compone de los siguientes capítulos:
    - En el Capítulo (4) se presenta una breve introducción de las diferentes derivaciones de ecuaciones maestras y EES que existen en la literatura, tanto para interacciones Markovianas como no-Markovianas, con el objeto de contextualizar aquellas que en particular se tratan en este trabajo.
    - En el Capítulo (5) nos centramos ya en el estudio de sistemas cuánticos abiertos con interacción no-Markoviana, y lo hacemos a lo largo de dos Secciones. En la Sección (5.1) estudiamos la eficiencia de algunas de las EESs existentes en la literatura, lo que es conocido como problema de sampleo. Ciertas EESs dan lugar a un conjunto de vectores de onda que tienen un peso más significativo que las soluciones de otras en el sampleo estocástico del operador densidad reducido. Mostramos para el modelo spin-boson que dicha mejora depende de las condiciones físicas del sistema total, particularmente de la temperatura del entorno. En la Sección (5.2), se discute el problema de generar ecuaciones maestras a partir de la ecuación de evolución del operador densidad reducido. Por un lado, cuando el estado inicial del entorno es el vacío, el propagador reducido da lugar a las ecuaciones de Schrödinger que habitualmente se encuentran

en la literatura, las cuales, tras hacer un promedio sobre los diferentes estados del entorno, reproducen el resultado de la ecuación maestra. Mientras que este caso ya ha sido tratado anteriormente en la literatura, nuestra aportación consiste en considerar un propagador reducido cuyo estado inicial es distinto del vacío, obteniendose una ecuación maestra para estados iniciales generales, y no necesariamente de decorrelación entre sistema y entorno. La derivación de tal ecuación maestra requiere de una generalización del Teorema de Novikov, que también es desarrollada en este trabajo.

- La Parte (III) contiene el mayor número de resultados de ésta tesis. En ella se deriva una teoría para FCM no-Markovianas, así como las ecuaciones de Heisenberg de movimiento de operadores del sistema.

  Comenzamos mostrando la utilidad de dichas FCM en el contexto de óptica cuántica, donde se emplean para el cálculo de cantidades tales como el espectro de emisión o la estadística de fotones emitidos por un átomo. A continuación, la discusión se divide en dos capítulos:

  - En el Capítulo (8) se muestra que las FCM no-Markovianas obedecen una estructura jerárquica cuando no se establece ninguna aproximación. Para ser más exactos, se encuentra que las funciones de correlación de un tiempo (o valores medios cuánticos), dependen de funciones de correlación a dos tiempos, mientras que las correlaciones a dos tiempos dependen de funciones de correlación a tres tiempos. La estructura jerárquica se extiende hasta funciones de correlación de órdenes superiores, de modo que, en general, las funciones de correlación de N-tiempos dependen de funciones de correlación de $N+1$-tiempos. Aunque este es un resultado formal que no puede ser empleado a efectos computacionales, su derivación resulta ser una forma sistemática de obtener las ecuaciones para funciones de correlación generales a N-tiempos. Dichas ecuaciones pueden llegar a ser últiles desde el punto de vista práctico una vez rota la dependencia con correlaciones de orden superior.
  - En el Capítulo (9) se asume la aproximación de acoplamiento débil para romper la jerarquía y derivar ecuaciones para funciones de correlación a N-tiempos, siempre hasta segundo orden en el parámetro perturbativo. Esto nos permite mostrar que el TCR no se aplica para interacciones de tipo no-Markoviano.

- En la Parte (IV), se aplican algunas de las ecuaciones presentadas a lo largo de este trabajo a un sistema de dos niveles immerso en un campo de radiación en un material de banda fotónica. La discusión se divide nuevamente en dos capítulos:

  - En el Capítulo (11) se presenta un modelo apropiado para el problema. Mientras que el Hamiltoniano corresponde a un átomo de dos niveles dipolarmente acoplado al campo de radiación, y por tanto tiene la misma forma que el Hamiltoniano general presentado en el Capítulo (1), presentamos aquí nuevas aportaciones en la caracterización de la función de correlación. Para tal fin, proponemos un nuevo modelo de relación de dispersión del campo que sigue la estructura periódica propia de un campo de radiación en un CF. Una vez calculada la función de correlación, es posible obtener el ruido correspondiente.
  - Ambas cantidades (función de correlación y ruido) se emplean en el Capítulo (12) para evaluar valores medios de algunos operadores del sistema a través de la EES. En primer lugar, mostramos que el esquema estocástico es equivalente a la ecuación maestra tradicionalmente empleada para tratar este tipo de sistemas. En segundo lugar, mostramos que la función de correlación que proponemos da lugar a los fenómenos físicos previamente estudiados en la literatura. Finalmente calculamos algunas FCM del sistema.

- En la Parte (V) se establecen algunas conclusiones y se definen perspectivas para trabajos futuros.

Al final de la tesis se incluyen una serie de apéndices, que aunque no son necesarios para seguir el trabajo, completan algunos de los cálculos y conceptos descritos.

18.2 RESUMEN DE LA PARTE I

18.2.1 Capítulo 1: Sistemas cuánticos abiertos no-Markovianos.

En este capítulo se presentan los modelos generales de Hamiltoniano que describen los sistemas tratados en la tesis. Se trata en particular de sistemas cuánticos abiertos en los que la interacción con los grados de libertad del entorno, que además se supone descrito a través de un conjunto de osciladores armónicos, es de tipo lineal. Se explican además en qué tipo de sistemas aparece interación de tipo no-Markoviano, efectuándo una descripción cualitativa de la misma basada en la densidad de estados fotónica.

La dinámica de un sistema cuántico abierto se describe habitualmente considerando que éste es parte de un sistema total mayor, el cuál está aislado erspecto al resto del mundo. El Hamiltoniano del sistema total se denota como $H_{tot} = H_S + H_B + H_I$, donde H_S es el Hamiltoniano del sistema cuántico abierto (a partir de ahora referido tan solo como **sistema**), H_B el Hamiltoniano de su entorno, y H_I es el Hamiltoniano de interacción entre sistema y entorno.

Cuando el entorno es grande, su escala de evolución temporal es en general pequeña en comparación con las escalas de tiempo relevantes del sistema. La escala de tiempo del entorno se caracteriza por el tiempo de correlación τ_c, que es el empleado por el mismo en recobrarse de la interación con el átomo. Del mismo modo, la escala de evolución del sistema es caracterizada por el tiempo T_A que es el que tarda en relajar al equilibrio una vez que es puesto en contacto con el entorno. Existen ciertas situaciones en las que la separación de las escalas temporales es tan grande que τ_c es prácticamente cero en comparación con T_A. Este tipo de interacciones, que pueden ser tratadas con la denominada aproximación Markoviana, dan lugar a una dinámica del sistema que es local en el tiempo, es decir, que no depende de la historia de la evolución. En otras situaciones el tiempo de correlación del entorno es del orden de T_A, lo que podría influír significativamente en la dinámica del sistema haciendose necesario un tratamiento no-Markoviano de la interacción. Las interacciones no-Markovianas se dan en múltiples contextos, entre los que podemos destacar los siguientes,

- En física del estado sólido los efectos no-Markovianos son especialmente visibles a bajas temperaturas. Uno de los modelos más comúnmente empleados es el de Caldeira and Legget [20, 22], que describe un oscilador armónico linealmente acoplado a través de su coordenada de desplazamiento q a un entorno o baño, el cual es descrito a su vez por un conjunto de osciladores armónicos. En muchos sistemas físicos y químicos, la coordenada generalizada q viene asociada a un potencial efectivo que tiene dos mínimos bien diferenciados y situados en la misma energía. En tal caso, ya que dicho sistema solo consta de dos estados estables, el espacio de Hilbert del sistema se reduce a un espacio bidimensional. Esta situación, que es descrita por el denominado modelo spin-boson, se encuentra en numerosos ejemplos, como en el movimiento de defectos en una red cristalina, en el *tuneleo* de partículas ligeras en metales, y en ciertos tipos de reacciones químicas que incorporan procesos de transferencia electrónica (ver or ejemplo [22] así como sus referencias).

- En **óptica cuántica** numerosos efectos no Markovianos están presentes en los procesos de emisión y absorción de la luz, en particular cuando el campo de radiación se encuentra en un entorno estructurado. Entre dichos entornos estructurados destacan en especial las cavidades cuánticas [23, 24, 25, 26], y los materiales de banda fotónica (MBF), que presentan una periodicidad en el índice de refracción [27, 28].

- Los efectos no Markovianos surgen igualmente en la dinámica de los **condensados Bose-Einstein** (CBE). En éstos sistemas, los átomos se encuentran atrapados en su estado fundamental, de donde son extraídos a través de una doble transición laser a un estado final excitado, generandose de este modo un láser atómico. Como ejemplo particular de comportamiento no-Markoviano, el número de ocupación de los átomos en el estado fundamental presenta una serie de oscilaciones que pueden ser interpretadas como un síntoma de interferencia cuántica, y que está en clara diferencia con la Regla de Oro de Fermi que predice decaimiento exponencial [30, 31, 32].

A lo largo de la tesis se estudian principalmente dos tipos de sistemas: (a) El modelo spin-boson válido para interacciones de un sistema de dos niveles con cualquier reserva bosónica (ya sea de fotones o de fonones) bajo ciertas condiciones fenomenológicas. (b) Un átomo acoplado a un campo de radiación con interacción dipolar.

Dado que las ecuaciones dinámicas que aquí tratamos son válidas para un modelo general de Hamiltoniano de interacción lineal sistema-entorno, la metodología podría ser aplicada a otros problemas, tales como la dinámica de condensados de Bose-Einstein.

El capítulo comienza presentando el modelo de Caldeira y Legget, así como el modelo Spin-Bosón al cuál se reduce bajo ciertas condiciones [20, 22, 33, 34]. En este esquema, el Hamiltoniano de interacción H_I es proporcional a SB, donde B es un operador que pertenece al espacio de Hilbert del entorno, y $S = q$ es el operador de acoplamiento del sistema. El operador de acoplamiento del entorno $B \propto \sum_\lambda g_\lambda \mathcal{F}(a_\lambda, a_\lambda^\dagger)$, donde g_λ son las constantes de acoplamiento del sistema con cada uno de los osciladores armónicos λ que describen el entorno, y $\mathcal{F}(a_\lambda, a_\lambda^\dagger)$ es una función determinada de los operadores de creación y de destrucción $a_\lambda^\dagger$ y a_λ.

El Hamiltoniano lineal de interacción propuesto en el modelo de Caldeira-Legget puede ser generalizado y expresado como una suma sobre muchos operadores de acoplamiento de baño y sistema, es decir i.e. $H_I = \sum_\beta S_\beta B_\beta$. Particularmente, el Hamiltoniano de interacción entre un campo bosónico y un campo fermiónico posee dicha forma. Un ejemplo de este tipo de sistemas es un átomo (cuyos electrones forman el campo fermiónico), en contacto con el campo de radiación (el cual es bosónico). Del mismo modo que en el modelo de Caldeira-Legget, se encuentra que los operadores B_β poseen la forma $B_\beta \propto \sum_\lambda g_{\lambda,\beta} \mathcal{F}_\beta(a_\lambda, a_\lambda^\dagger)$. No obstante, en contraste con el modelo anterior, en este sistema se conocen las dependencias exactas de los operadores de acoplamiento $g_{\lambda,\beta}$.

Se introduce a continuación una nueva notación, que consiste en expresar el Hamiltoniano de interacción en término de los denominados operadores de Lindblad $\{L_\lambda\}$, que son combinaciones de los operadores de acoplamiento del sistema $\{S_\beta\}$. El Hamiltoniano del sistema total en su forma Lindblad se emplea como modelo general a partir del cual se desarrollan la mayor parte de las ecuaciones empleadas en ésta tesis en la descripción de la dinámica de un sistema cuántico abierto. Existen dos razones fundamentales para el uso de la forma Lindblad: la primera es que cuando la interacción es Markoviana da lugar a una ecuación maestra que preserva la positividad del operador densidad reducida, y la segunda es que es uno de los Hamiltonianos más comunmente empleados para el estudio de sistemas cuánticos abiertos.

Como ya se ha mencionado anteriormente, una cantidad fundamental para caracterizar la influencia del entorno en el sistema es la función de correlación del mismo, $\alpha(t)$, ya que aparece en todas las ecuaciones dinámicas del sistema, y además determina el tiempo de memoria o tiempo de correlación del entorno tras la interacción τ_c. La función de correlación es proporcional a la suma del cuadrado de las constantes de acoplamiento del sistema con cada oscilador armónico, $\alpha(t) \propto \sum_\lambda g_\lambda^2 \mathcal{P}(t, \omega_\lambda)$, donde $\mathcal{P}(t, \omega_\lambda)$ es una determinada función que no depende del modelo en cuestión.

En el continuo, esta suma se transforma en una integral cuyo kernel es la llamada función densidad espectral, $J(\omega)$, de tal modo que $\alpha(t) = \int d\omega J(\omega)\mathcal{P}(t,\omega)$. Dado que $\mathcal{P}(t,\omega)$ tiene la misma forma para cualquier sistema, la función densidad espectral contiene la misma información que la función de correlación, caracterizando de forma equivalente la interacción del entorno sobre el sistema.

Tratamos en la Sección (1.3) algunos aspectos concernientes a la función de correlación y a la densidad espectral, en especial las características que determinan que la interacción sea Markoviana o no-Markoviana. Existen dos métodos distintos para derivar la función de correlación.

El primero, es conocido como *microscópico* ya que se basa en el conocimiento de la forma de las constantes de acoplamiento. En este capítulo se ilustra el método empleando las constantes de acoplamiento que caracterizan la interacción de un sistema de dos niveles con el campo electromagnético en el vacío, para derivar una función de correlación típicamente Markoviana. Se encuentra que en dicha interacción, la función $J(\omega)$ varía suavemente en frecuencias en comparación con el ritmo de emisión espontánea del átomo Γ, de modo que puede ser considerada aproximadamente constante. En los siguientes capítulos se hacen derivaciones más complicadas de funciones de correlación correspondientes a átomos en entornos estructurados. Como ya se ha mencionado en la introducción, estos sistemas son típicamente no-Markovianos, por lo que la densidad espectral varía en un rango de frecuencias comparable con Γ y no debe ser aproximada como constante.

El segundo método es empleado cuando no se conoce la forma exacta de las constantes de acoplamiento, tal y como ocurre en el modelo de Caldeira y Legget. La función espectral se ha de construír ahora acorde con diversos argumentos de tipo *fenomenológico*. Se presenta en este capítulo la derivación empleada para el cálculo de la $J(\omega)$ empleada en el modelo spin-boson que será integrado posteriormente.

18.2.2 Capítulo 2: El operador reducido del sistema

Presentamos el propagador reducido del sistema, que es la herramienta básica con la que se van a derivar gran parte de las ecuaciones dinámicas de esta tesis. El propagador reducido es la representación del operador de evolución unitario del sistema total en la base de estados coherentes Bargmann del baño. Se trata de un objeto que propaga temporalmente el estado cuántico del sistema dados un determinado estado inicial y final del entorno. La ecuación de evolución del propagador, que constituye uno de los resultados de esta tesis, depende de dos funciones temporales $z_{i,t}$ y $z_{i+1,t}$ que dependen de los números cuánticos que determinan respectivamente dichos estados inicial y final del entorno.

Por tratarse de una interacción de tipo Markoviano, la ecuación de evolución del propagador del sistema, ecuación (2.40), es *abierta*. Ello significa que no depende únicamente del propagador que se está evolucionando, sino de un objeto que pertenece al espacio de Hilbert del sistema total. Si queremos expresar la ecuación en espacio de Hilbert del sistema, es preciso introducir una relación de cierre del baño en dicho objeto, que queda transformado en una suma sobre las trajectorias de otros propagadores. Esta nueva manera de espresar la ecuación muestra que, cuando no se establece ninguna aproximación, la dinámica del propagador reducido del sistema estaá enmarañada con el resto de los propagadores. Dado que dicho enmarañamiento solo existe a lo largo de un tiempo τ_c, es propio tan solo de interacciones de tipo no-Markoviano. Al ser abierta, la ecuación (2.40) es difícil de manejar desde el punto de vista computacional, y solo nos servirá de base para, en el Capítulo (8), derivar la jerarquía de ecuaciones que obedecen las funciones de correlación.

El empleo para fines prácticos de la ecuación del propagador requiere transformar la anterior ecuación en una ecuación *cerrada*, que perteneciendo al espacio de Hilbert del sistema sólo dependa del propagador que se está evolucionando. La manera de obtener dicha ecuación es aplicando alguna hipótesis o aproximación sobre el sistema. En todas las hipótesis coincide el hecho de que el objeto o elemento de matriz que hace abierta la ecuación es expresado en términos de un determinado operador O multiplicado por el propagador que se está evolucionando. Destacamos la hipótesis de consistencia o expansión, la hipótesis perturbativa, y la aproximación que consiste en considerar que en el problema que se trata la interacción es casi Markoviana. A lo largo de la tesis, empleamos fundamentalmente la aproximación perturbativa, que consiste en asumir que la energía de la interacción, expresada a través de su Hamiltoniano, es pequeña en magnitud en comparación con la energía del sistema libre. En esta aproximación el operador O se calcula a través de una serie de Taylor sobre un parámetro perturbativo g. Dicho parámetro, también conocido como constante de acoplamiento, regula la diferencia en magnitud entre el Hamiltoniano de interacción y el Hamiltoniano libre. Mostramos igualmente como el parámetro g está relacionado también con τ_c.

El propagador reducido del sistema es fundamental para la obtención de las cantidades que describen su dinámica, ya sean valores medios o funciones de correlación múltiples. No obstante, como ya se ha mencionado, es condición indispensable para ello el poder efectuar el promedio sobre los distintos estados iniciales y finales posibles del entorno. A lo largo de esta tesis vamos a emplear dos tipos de promedio:

- De tipo estocástico. Consiste en considerar dicho promedio como un muestreo de tipo Montecarlo, en el cual se sortean estados aleatorios del entorno acorde con su distribución. La ecuación del propagador pasa a ser una ecuación estocástica de Schrödinger. La consideración del propagador como estocástico ya fue efectuada en [41], pero entonces solo existía la ecuación dinámica para un entorno inicialmente en el vacío.

- De tipo analítico. Consiste en efectuar la suma sobre estados del baño analíticamente, acorde con el denominado Teorema de Novikov. Constituye un resultado de esta tesis la extensión de dicho teorema necesaria para tratar promedios con propagadores en los que el estado inicial del baño no es el vacío.

En las Partes (II) y (III) se emplea la ecuación cerrada (2.52) para derivar la ecuación maestra, así como las ecuaciones de funciones de correlación múltiples hasta segundo orden en el parámetro perturbativo. Cuando considera el vacío como el estado inicial del entorno, por lo que $z_{i+1,t} = 0$, la integración de la ecuación de evolución del propagador da lugar el operador densidad reducido con condición inicial $\rho_s(0) = Tr_S\left(\rho_{tot}(0)\right) = Tr_S\left(|\psi_0\rangle\langle\psi_0| \otimes |0\rangle\langle 0|\right)$, una vez que el promedio sobre el estado final del entorno z_i se ha efectuado. Como hemos dicho, este procedimiento ya ha sido descrito anteriormente en la literatura [54, 55, 6]. Para un estado inicial del entorno distinto del vacío, $z_{i+1} \neq 0$, el propagador reducido puede ser empleado para calcular una nueva ecuación maestra adecuada para condiciones iniciales generales de sistema y entorno, así como funciones de correlación múltiples.

18.3 RESUMEN DE LA PARTE II: VALORES MEDIOS CUÁNTICOS.

18.3.1 Capítulo 4: Introducción

Tradicionalmente, la investigación de sistemas cuánticos abiertos quedaba centrada en el problema de determinar la evolución del operador densidad reducido a través de unas ecuaciones de evolución $\dot{\rho}_s$ denominadas **ecuaciones maestras**, pues el conocimiento de ρ_s en cada instante, permite calcular el promedio de cualquier observable A del sistema a través de la expresión típica

$$\langle A(t)\rangle = Tr_s\{\rho_s(t)A\}. \tag{18.1}$$

Estas ecuaciones maestras son el equivalente cuántico a las ecuaciones de evolución de la distribución de probabilidad clásica que ya hemos mencionado en la introducción.

En años recientes, se ha desarrollado un método distinto para el estudio de sistemas cuánticos abiertos, que consiste en resolver la dinámica del sistema a través de soluciones $|\psi_t(z^*)\rangle$ de una ecuación de Schrödinger que ahora es estocástica debido a la interacción con el medio. El carácter estocástico de $|\psi_t(z^*)\rangle$ se imprime a través de la dependencia con un cierto ruido z_t^* que caracteriza el efecto del medio sobre el sistema. Más adelante trataremos de dar una explicación más concreta de la procedencia de esta variable y de su conexión con el estado del medio. En ocasiones adoptaremos la terminología comúnmente empleada de referirnos a las soluciones $|\psi_t(z^*)\rangle$ como *trayectorias cuánticas* [52].

Las **ecuaciones estocásticas de Schrödinger** tienen como propiedad el que un promedio en la variable z^* al conjunto estadístico de sus soluciones a un tiempo t, $|\psi_t(z^*)\rangle$, definiendo este promedio como $M[| \psi_t(z^*)\rangle\langle\psi_t(z)\ |]$ da lugar a la matriz densidad reducida a dicho tiempo:

$$\rho_s = M[|\ \psi_t(z^*)\rangle\langle\psi_t(z)\ |]. \tag{18.2}$$

Esta relación a menudo se dice que representa un *revelado* de la dinámica del operador densidad reducido, y como veremos más adelante, entraña también un *desenmarañamiento* efectivo de la dinámica sistema-entorno.

El esquema estocástico presenta diversas ventajas respecto al tradicional representado por las ecuaciones maestras.

- En las ecuaciones maestras, la tarea consiste en determinar la dinámica del operador densidad reducido ρ_s, que es una matriz $N \times N$, siendo N la dimensión del espacio de Hilbert del sistema abierto. En general estas ecuaciones solo pueden ser determinadas de forma aproximada, o empleando modelos simples para el sistema y su entorno. Incluso cuando es posible derivar una evolución cerrada para ρ_s, si queremos calcular la evolución de sistemas cuánticos con un número de dimensiones grande, nos encontraremos con problemas numéricos importantes a la hora de manejar matrices cada vez mayores.

  El esquema estocástico supone resolver en cada trayectoria una solución $|\psi_t(z^*)\rangle$ de dimensión N, por lo que un aumento de grados de libertad no resulta tan grave como en el caso de las ecuaciones maestras.

  No obstante, como veremos más adelante, dada una determinada dimensión N, el metodo de las ecuaciones estocásticas solo resulta eficaz numericamente si el conjunto de trayectorias que se escogen para efectuar el promedio (18.2) es estadísticamente significativo. Como veremos más adelante, la estadadística escogida para las trayectorias dará lugar a distintos tipos de ecuaciones estocásticas de Schrödinger, y el objetivo principal de este trabajo será justificar en que condiciones son más eficaces unas ecuaciones u otras.

- Aparte de las ventajas numéricas, las ecuaciones estocásticas de Schrödinger presentan otras propiedades importantes. Principalmente, proporcionan mayor información de la dinámica del sistema cuántico abierto que las ecuaciones maestras, en las que los grados de libertad del entorno son eliminados mediante una traza y, por tanto, permanecen sin ser observados. En las ecuaciones estocásticas, la dinámica de los grados de libertad del baño son una parte explícita de la descripción. En concreto, los vectores de estado del sistema dependen del estado del baño, por lo que se dice que la ecuación estocástica describe en realidad una dinámica *condicionada*.

Podemos distinguir dos tipos básicos de esquema estocástico para la evolución de la función de ondas en imagen de Schrödinger: En el primero la evolución de dicha función es determinista hasta que se ve interrumpida por procesos de salto estocásticos que la proyectan instantáneamente a un estado cuántico. En el segundo esquema la evolución es gobernada a través de una variable estocástica continua[2], que actúa en cada momento infinitesimal de la dinámica del sistema.

---

[2] La variable estocástica, se denomina en este caso *proceso Wiener* [51]

Al primero de los esquemas estocásticos descritos pertenece el denominado **método de saltos cuánticos**. Éste corresponde a una dinámica del sistema condicionada por una sucesión continua de medidas del número de fotones del entorno. Debido a que sistema y entorno están entrelazados, una medida sobre el segundo afecta a la dinámica del primero. Así, en el caso de un átomo inmerso en un campo de radiación, podemos saber si se encuentra en el estado excitado o en el fundamental en función de si hemos medido o no un fotón en el baño. Debido a que el resultado de esta medida es estocástico, si repetimos el procedimiento sucesivas veces (ya sea desde una misma condición inicial o desde un conjunto de ellas), obtendremos un conjunto estadístico de trayectorias. El promedio sobre el mismo nos permite obtener el resultado tradicionalmente obtenido por la ecuación maestra para el operador densidad reducido del sistema, esto es, un decaimiento exponencial de la probabilidad de ocupación del estado excitado. Este esquema tiene como principal inconveniente el que sólo es aplicable a sistemas cuya interacción con el baño es de tipo Markoviano, es decir, aquellos en los que la escala temporal de relajación del entorno es mucho menor que la del sistema.

Al segundo esquema de proceso estocástico, que da lugar a una ecuación de Schrödinger continua y difusiva, corresponde el llamado **método de difusión del estado cuántico** (QSD), propuesto por Gisin [83] y más tarde desarrollado también por Percival [88], y que permite, a diferencia de los saltos cuánticos, generar ecuaciones estocásticas aptas para el caso en el que la interacción con el baño sea tipo no-Markoviano. En el caso Markoviano en el que es posible establecer medidas continuas sobre el entorno sin alterarlo, las trayectorias difusivas corresponden al resultado de experimentos de detección homidínica y heterodínica [93, 94].

Es de señalar que las ecuaciones estocásticas de Schrödinger difusivas, pasando a imagen de Heisenberg, dan lugar a ecuaciones estocásticas de evolución de operadores. Calculando por ejemplo la ecuación de evolución del operador posición de una partícula cuántica sometida a movimiento Browniano, obtendremos el equivalente cuántico de la ecuación de Langevin.

En este estudio se emplearán ecuaciones estocásticas de Schrödinger obtenidas en el marco del *método de difusión del estado cuántico* y se aplicarán al caso más general no-Markoviano.

18.3.2 Capítulo 5: Valores medios cuánticos de un sistema con interacción no-Markoviana

En el anterior capítulo se discutieron las distintas derivaciones de ESS que aparecen en la literatura, tanto para interacciones Markovianas como no Markovianas, así como la interpretación de las primeras en términos de medida continua. En este capítulo se particulariza a las ESS no-Markovianas derivadas por el método de proyección de Feshbach [1, 37], así como las derivadas a través de los propagadores reducidos cuando éstos son considerados como estocásticos [3, 4, 41].

La motivación del capítulo es doble: Primero, estudiar y comparar las distintas ESS existentes en la literatura, con el objeto de probar su equivalencia con la ecuación maestra, así como su eficiencia. Tal eficiencia tiene que ver con el número de trajectorias necesarias para, a través del promedio estocástico, obtener el operador densidad reducido, así como con el tiempo empleado en la integración de cada una de las mismas. Segundo, emplear el propagador reducido para derivar ecuaciones maestras correspondientes a distintas condiciones iniciales.

Acorde con estas dos metas, el capítulo se divide en dos Secciones

En la Sección (5.1), se estudia la evaluación de promedios cuánticos a través de un *sampleo numérico de las distintas trajectorias estocásticas*. Pese a no existir por el momento ninguna interpretación de las EES no-Markovianas en término de experimentos de medida continua, su utilidad no solo está relacionada con dicha interpretación. Incluso no dando ninguna interpretación física al estado que se evoluciona, la formulación de trajectorias estocásticas constituye una herramienta eficiente desde el punto de vista numérico en comparación con las ecuaciones maestras. Dicha eficiencia depende de dos factores principales: 1) que el número de grados de libertad del sistema sea grande, y 2) que el muestreo de la EES sea bueno, de forma que solo sea necesario un número pequeño de trajectorias estocásticas para efectuar los promedios. El primer factor es intrínseco al sistema particular que se estudie, mientras que el segundo depende del modelo de ecuación estocástica elegido. En esta primera Sección tratamos de responder a la pregunta de cual es el modelo de ecuación que mejora el muestreo, y cuándo dicha mejora es suficientemente significativa como para decidirse por tal modelo. Estudiando en particular un modelo spin-boson, encontramos que la temperatura del medio es un factor fundamental que considerar a la hora de seleccionar el modelo adecuado de EES, ya que dicha temperatura altera de manera significativa la distribución de estados del sistema y, por tanto, la estadística del ruido.

En la Sección (5.2), nos centramos en el uso de los propagadores reducidos para calcular valores medios a través de la ecuación maestra del operador densidad reducido. Tal y como fue introducido en el Capítulo (2), cuando el promedio de los propagadores reducidos no se hace mediante el método estocástico sino analíticamente, dichos propagadores pueden ser empleados para derivar ecuaciones maestras. Señalamos a continuación dichas condiciones iniciales, así como las correspondientes ecuaciones,

- El sistema y el entorno están inicialmente decorrelacionados, de modo que

  $$\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0). \tag{18.3}$$

  Se consideran aquí dos casos para la matriz densidad del baño, ρ_B correspondiente al estado del vacío, y ρ_B correspondiente a un estado termal. La ecuación maestra correspondiente al primer caso ya había sido obtenida en la literatura mediante el promedio analítico de propagadores reducidos. Sin embargo, la segunda ecuación no había sido obtenida mediante dichos propagadores, sino a través de un procedimiento distinto [54]. La razón es que cuando el baño es térmico se precisa el propagador reducido en el que el estado inicial no es el vacío, objeto que como hemos dicho es introducido por vez primera en este trabajo.

- El sistema y el entorno están inicialmente correlacionados,

  $$\rho_{tot}(t_0) = \rho_s(t_0) \otimes \rho_B(t_0) + \rho_{correl}(t_0), \tag{18.4}$$

  donde el último término ρ_{correl} corresponde a una cierta correlación inicial. En estas circunstancias es de nuevo precisa la utilización de un propagador reducido en el que el estado inicial el baño no sea el vacío. Gracias al mismo, y a través de un promedio analítico, derivamos la ecuación maestra que evoluciona el operador densidad reducido.

18.4 RESUMEN DE LA PARTE III: FUNCIONES DE CORRELACIÓN MULTITEMPORALES

18.4.1 Capítulo 7: Introducción y motivación

Hay situaciones en las que los valores medios de los observables del sistema no son suficientes para describir las características esenciales de su comportamiento físico. Podemos encontrar ejemplos de ésto en física estadística y en espectroscopía, campos en los que se estudia la respuesta del sistema a un campo magnético externo.

En este capítulo motivamos el uso de las funciones de correlación múltiples en el campo de la óptica cuántica, y lo hacemos con dos ejemplos diferentes. En primer lugar, las correlaciones a dos tiempos del campo electromagnético emitido por el átomo son necesarias para el estudio de sus propiedades espectroscópicas. Mostrando cuál es la relación de dicha correlación con la correlación de operadores del sistema para el caso no-Markoviano, vemos que el espectro puede ser calculado a través de dichas correlaciones. En segundo lugar, las funciones de correlación a dos tiempos del número de fotones emitidos permiten la descripción de un efecto púramente mecano cuántico, que es el denominado *anti-bunching* fotónico. Dichas correlaciones pueden ser expresadas en función de una correlación a cuatro tiempos de operadores del sistema, lo que muestra nuevamente la utilidad de una teoría para el cálculo de funciones de correlación múltiples.

18.4.2 Capítulo 8: Jerarquía de FCM non-Markovianas

Se deriva en este capítulo la **jerarquía** de ecuaciones que obedecen formalmente las funciones de correlación múltiples no-Markovianas cuando no se establece ninguna aproximación. Se emplean dos métodos distintos en el desarrollo de dichas ecuaciones: el primero, descrito en la Sección (8.1), está basado en utilizar propagadores reducidos del sistema, mientras que el segundo, explicado en la Sección (8.2), está basado en el uso de las ecuaciones de Heisenberg de operadores del sistema.

La estrutura jerárquica consiste en lo siguiente: la ecuación de evolución para funciones de correlación de un tiempo (es decir, promedios cuánticos), depende de funciones de correlación a dos tiempos. Y más aún, la ecuación de evolución de dos tiempos depende de funciones de correlación de tres tiempos. Lo mismo ocurre con la ecuación de evolución de correlaciones a tres tiempos, que depende de funciones de correlación a cuatro tiempos. En resumen, la evolución de funciones de correlación no-Markovianas de N-tiempos de operadores del sistema depende de funciones de correlación de $N+1$-tiempos cuando no se ha efectuado ninguna aproximación.

La jerarquía solo ocurre en interacciones de tipo no-Markoviano, puesto que desaparece cuando la función de correlación del baño, $\alpha(t)$, es proporcional a una delta, como es propio de un baño Markoviano. Un uso práctico de las ecuaciones de evolución de funciones de correlación multitemporales pasa por romper la jerarquía y eliminar la dependencia con funciones de correlación de orden superior mediante el uso de alguna hipótesis. Esta idea es llevada a cabo en el siguiente capítulo, en el cual se considera una aproximación de acoplamiento débil hasta segundo orden en el parámetro de acoplamiento.

18.4.3 Capítulo 9: FCM no-Markovianas hasta segundo orden en el parámetro perturbativo

Se presentan en este capítulo tres métodos distintos para derivar las funciones de correlación multitemporales hasta segundo orden en el parámetro perturbativo.

El primero, descrito en la Sección (9.1), es esencialmente *numérico*, y consiste en hacer el promedio al conjunto de distintas trajectorias estocásticas. Estas trajectorias se obtienen empleando la ecuación a segundo orden del propagador reducido (7.50), en la cual $O(z_{i+1}z_i^*, t, \tau) = V_{t-\tau}L$.

Los otros dos métodos consisten en derivar el conjunto de ecuaciones diferenciales que obedecen las FCM: En la Sección (9.2.1) se obtiene dicho conjunto haciendo una expansión perturbativa del propagador reducido, y luego realizando el promedio *analítico* sobre las variables medioambientales z_{i+1} y z_i. En la Sección (9.2.2), se presenta un tercer método consistente en aplicar la hipótesis perturbativa a segundo orden a la jerarquía de ecuaciones de evolución derivada en el anterior capítulo. Como ya hemos notado, para utilizar la jerarquía de ecuaciones computacionalmente, y no solo como una derivación formal, debe romperse la dependencia con correlaciones de órdenes superiores. En este capítulo hacemos esto empleando una hipótesis perturbativa a segundo orden diréctamente en la correlación a tiempo N que queremos calcular, de modo que desaparece su dependencia con correlaciones a tiempo $N+1$.

18.5 PARTE IV: DINÁMICA DE UN SISTEMA DE DOS NIVELES EN UN MATERIAL DE BANDA FOTÓNICA

18.5.1 Capítulo 11: El modelo

Cuando la luz penetra en un medio con diferente índice de refracción, puede ser reflejada y refractada. Mientras que la luz reflejada regresa a través del medio incidente, la luz refractada penetra a través del nuevo medio y sufre un cambio de velocidad, el cuál a su vez es responsable de una variación en su dirección de propagación. La luz que atraviesa un medio homogéneo en el que no hay variación del índice de refracción no será ni reflejada ni refractada en ninguna dirección.

Supongamos ahora que construímos un material en el que el índice de refracción varía solo en una dirección. En ese caso, solo la luz que se propaga en esa dirección será reflejada y refractada. Considerando además que el cambio en el índice de refracción es periódico, el proceso de reflexión se repetirá cada vez que la luz sufre un nuevo cambio en el índice de refracción. Este tipo de materiales puede ser construído alternando capas de alto índice de refracción y de anchura a con capas de bajo índice y anchura b. Gracias a la periodicidad, los rayos de luz son reflejados de forma coherente, produciéndose entre ellos fenómenos de interferencia. Un máximo en la reflexión se forma cuando los rayos reflejados interfieren constructivamente, lo que ocurre cuando se verifica la condición de Braag [110].

Para aquellos rayos que penetran perpendicularmente a las capas (esto es, en la dirección de cambio del índice de refracción), la condición de Braag está dada por

$$2a = \lambda_0, \tag{18.5}$$

donde λ_0 es la longitud de onda del vacío. Los rayos de luz que penetran perpendicularmente a las capas, y cuya longitud de onda esté dada por la relación anterior, son reflejados y no aparecen en el cristal fotónico. Esto da lugar a la formación de un gap en la densidad de estados fotónica correspondiente a las frecuencias de los modos reflejados.

Siguiendo un procedimiento análogo al anteriormente descrito, es posible fabricar un gap $3D$ generando una estrutura dieléctrica perióndica en las tres dimensiones. De este modo, la luz que incide en el material con una frecuencia relacionada con la periodicidad de la red es reflejada fuera del cristal independientemente del ángulo de incidencia.

Este tipo de cristales son conocidos como materiales de banda fotónica (también cristales fotónicos), y fueron inicialmente propuestos por John y Yablonovitch [12, 13, 111] como medios para localizar y atrapar la luz en un material [13], y para producir la completa inhibición de la emisión espontánea a lo largo de un amplio rango de frecuencias [12].

Otra forma de entender la estructura de bandas de un cristal fotónico es considerandolos como el análogo óptico de los cristales semiconductores para electrones. En lugar de una red de átomos periódicamente ordenada que refleja a los electrones modificando su relación energía momento, un material fotónico está compuesto de una red periódica en el índice de refracción. En cristales semiconductures, los autovectores del electrón en presencia de la red periódica difieren de aquellos propios del vacío, de modo que para ciertos autovalores no existe un autovector correspondiente. Del mismo modo, en un cristal fotónico existen ciertos valores de frecuencia para los que no hay un vector de ondas o modo del campo correspondiente. De esta forma, la relación entre ambas magnitudes, también conocida como relación de dispersión, presenta una estructura especial en la que las bandas de frecuencias permitidas (para las que si existen modos del campo), están separadas por bandas de valores de frecuencia prohibidos o gaps.

Como ya se ha mencionado, la densidad de estados del campo de radiación presenta regiones de frecuencia en las que es cero, correspondientes a los gap, separadas por zonas donde es no nula, correspondientes a las bandas, en las que puede llegar a tener valores incluso más altos que en el vacío. Además, la densidad de estados fotónicos varía rápidamente en el borde del la banda que limita con el gap, lo que implica que el tiempo de correlación de las fluctuaciones del vacío no es despreciable en comparación con la escala de evolución temporal del sistema. Este factor hace inapropiada la aproximación Markoviana habitualmente empleada en óptica cuántica. La dinámica de un átomo excitado con frecuencia de resonancia cercana al eje del gap presenta algunas características particulares, que incluyen la inhibición de la emisión espontánea [112], una fuerte localización de la luz [13], la formación de estados enlazados átomo-fotón [113] y la inversión atómica en el estado estacionario [114].

Los materiales de banda fotónica han atraido una atención considerable tanto entre científicos como entre ingenieros, debido a sus muchas posibilidades y aplicaciones. En este trabajo, nos ocupamos en particular de dar una descripción teórica de algunos de los aspectos de la dinámica de un átomo de dos niveles en tal tipo de materiales, incluyendo alguno de los efectos arriba mencionados. Para ello aplicaremos algunas de las ecuaciones dinámicas desarrolladas en las Partes (II) y (III) a tal sistema.

Comenzamos generando un modelo para describir el sistema. En el Capítulo (1) ya fueron obtenidos el Hamiltoniano de un átomo de dos niveles en contacto con un campo de radiación, así como las dependencias de las constantes de acoplamiento g_λ. También se mostró que la función de correlación del entorno $\alpha(t-\tau)$ puede ser construída con el conocimiento de tales constantes y de las frecuencias del correspondiente oscilador armónico ω_λ. Entre otros factores, las g_λ dependen de la relación de dispersión del campo. En este capítulo se propone un modelo particular para la relación de dispersión del campo en un material de banda fotónica, y se sigue el modelo de derivación microscópica propuesto en la Sección (1.3.1.1) para generar la función $\alpha(t-\tau)$ característica de tal tipo de campo. Tal y como se ve a lo largo de la tesis, dicha función es básica, ya que forma parte de todas las ecuaciones dinámicas que evolucionan tanto valores medios como funciones de correlación multitemporales de un sistema cuántico abierto. En la literatura han sido propuestas anteriormente algunas funciones de correlación del entorno [42]. No obstante, todas ellas presentan el problema de ser singulares en el origen, lo que las hace inapropiadas para generar el ruido z_t tal que el promedio de su autocorrelación, $\mathcal{M}[z_t z_\tau^*] = \alpha(t-\tau)$. La función de correlación que nosotros proponemos captura gran parte de los aspectos físicamente relevantes de las ya existentes, y además describe con mayor precisión que éstas el comportamiento a tiempos cortos. Por esta razón, no presenta una singularidad en el origen, siendo entonces apta para la generación del ruido que nos permite el empleo de un esquema estocático.

18.5.2 Capítulo 12: Promedios cuánticos y fluctuaciones.

Estudiamos ahora la dinámica de los valores medios, emplando una ecuación de Schrödinger estocástica. Con el objeto de verificar la validez de la formulación estocástica, estudiamos algunos de los fenómenos físicos que ocurren en un átomo dentro de un material de banda fotónica, como por ejemplo la aparición de población residual en el estado excitado a tiempos largos, el estado enlazado átomo-fotón, y la inversión de población que ocurre cuando además se le aplica al átomo un campo láser externo [6, 42].

Además de la ecuación estocástica, estudiamos las dos ecuaciones maestras perturbativas hasta segundo orden que fueron presentadas en el Capítulo (5): la ecuación convolucionada y la ecuación no convolucionada. Mostramos que ésta última, que además es la que se ha empleado en estudios previos, no preserva la positividad para determinados valores de los parámetros empleados, mientras que la no convolucionada preserva por construcción la positividad.

Finalmente, estudiamos algunas fluctuaciones del átomo de dos niveles. Tal y como se trató en el Capítulo (III), estos resultados podrían servir como punto de partida para el cálculo del espectro de emisión de dicho átomo. Del mismo modo, se podrían calcular funciones de correlación a cuatro tiempos, con el objeto de observar efectos como el anti-*bunching* fotónico. Como hemos mencionado anteriormente, estos dos fenómenos (espectro de emisión y anti-*bunching*) han sido ampliamente estudiados para el caso

Markoviano, pero no para interacciones no-Markovianas. Nuestro trabajo, por tanto, resulta un punto de partida prometedor para futuras investigaciones.

La formulación que presentamos en esta parte de la tesis para describir átomos en materiales de banda fotónica puede ser extendida para el estudio de sistemas más complejos, como por ejemplo átomos de más de dos niveles inmersos en estruturas fotónicas más complejas. Una formulación estocástica como la que hemos empleado resulta especialmente interesante para tratar átomos de más de dos niveles, puesto que como se ha explicado anteriormente la mejora computacional de dicha formulación respecto a la ecuación maestra resulta especialmente significativa cuando aumentan los grados de libertad del sistema en cuestión.

18.6 CONCLUSIONES

Hemos estudiado y derivado las herramientas necesarias para describir un sistema abierto no-Markoviano acoplado linealmente a un entorno de osciladores armónicos. Como ejemplo, hemos aplicado las ecuaciones a un átomo acoplado dipolarmente al campo de radiación existente en un CF. Recogemos aquí algunos de los resultados y conclusiones principales de esta tesis, tratando de dar una visión global del trabajo.

- Comenzamos introduciendo el propagador reducido, que evoluciona el estado del sistema condicionado a un estado inicial y final del entorno. El propagador reducido es el elemento de matriz del operador de evolución del sistema total en la base de estados coherentes Bargmann del entorno. Tanto el operador densidad reducido, como las FCM del sistema pueden ser expresados como un promedio Gaussiano de propagadores reducidos, que es realizado sobre los estados inicial y final del entorno. El promedio se puede efectuar de dos maneras: Primero, numéricamente, considerando un muestreo Montecarlo de la suma, de modo que los propagadores reducidos se convierten en propagadores estocásticos. Con este método el operador densidad reducido y las FCM se obtienen evolucionando diversas trajectorias estocásticas, y luego efectuando una suma sobre las mismas. Segundo, analíticamente, lo que permite la obtención de las ecuaciones de evolución del operador densidad reducido y de las FCM.

- Hemos estudiado el muestreo de distintos modelos de EES para obtener el operador densidad reducido. Mostramos en particular que las ecuaciones EES de tipo no lineal, que se caracterizan por tener una distribución dinámica para el ruido, presentan una mejora en el muestreo sólo cuando la temperatura ambiental es lo suficientemente alta. La razón de ello es que es en dichas condiciones cuando la función de distribución de los estados del entorno, que coincide con la función de distribución del ruido, evoluciona considerablemente debido a la interacción.

- A continuación, se ha empleado el propagador reducido para derivar distintas ecuaciones maestras a través de un promedio analítico. El resultado novedoso de esta tesis es el desarrollo de una extensión del teorema de Novikov para realizar tal promedio con propagadores en los que la condición inicial del entorno no es el vacío. Gracias a ello se ha derivado una nueva ecuación maestra que, en contraposición a las ya existentes, es apta para la descripción de problemas en los que el medio y el sistema cuántico no están inicialmente decorrelacionados.

- Hemos elaborado una teoría de funciones de correlación multitemporales no-Markovianas. Al ser éste uno de los resultados principales de la tesis, especificaremos más detalladamente los logros concernientes al mismo.
  - Comenzamos motivando el problema con la presentación de dos posibles aplicaciones de las FCM en óptica cuántica: el cálculo del espectro de emisión atómico (relacionado con una

función de correlación a dos tiempos de operadores del entorno), y el cálculo de la estadística de fotones (relacionado con una función de correlación a dos tiempos de los operadores del entorno, pero temporalmente ordenada). Señalamos la relación entre funciones de correlación de los operadores del entorno con funciones de correlación de los operadores del sistema para el caso no-Markoviano. Tal derivación solo existía, en nuestro conocimiento, para el caso Markoviano.

  - Derivamos la ecuación de evolución de las FCM empleando dos métodos: un primero basado en el uso de propagadores reducidos, y un segundo basado en en el uso de las ecuaciones de Heisenberg. Se muestra entonces que cuando no se emplea ninguna aproximación, las ecuaciones de evolución de las FCM se encuentran organizadas en una jerarquía, de modo que la evolución de funciones de correlación de N tiempos depende de funciones de $N+1$ tiempos. La jerarquía solo tiene uso formal, pues para ser empleada computacionalmente ha de romperse dicha dependencia.
  - Rompemos la jerarquía mediante el uso de una aproximación perturbativa hasta segundo orden en el parámetro de acoplamiento, obteniendo ecuaciones para funciones de correlación de N tiempos.
  - El hecho de que las funciones de correlación temporales no-Markovianas obedezcan a una estructura jerárquica cuando no hay aproximación, muestra ya que el teorema de regresión cuántico no es un resultado exacto para tal tipo de interacciones. No obstante, al derivar el conjunto de ecuaciones para FCM hasta segundo orden perturbativo, comprobamos que tampoco con dicha aproximación se cumple el teorema de regresión. Además, podemos expresar las ecuaciones de modo que queden explícitos los términos que hacen que dicho teorema no se cumpla, mostrandose así que, para el caso Markoviano, dichos términos desaparecen.
  - La teoría y procedimientos formulados se extienden en un Apéndice a funciones de correlación con ordenación temporal, las cuales son necesarias por ejemplo para el cómputo de estadística de fotones. Dichas funciones corresponden además a experimentos de medida continua sobre el sistema. En general, la teoría puede apliarse para cualquier ordenación temporal de los operadores que se correlacionan.
  - Asímismo, también la ampliamos para entornos con temperatura $T \neq 0$, en especial el caso de funciones de correlación a dos tiempos. Esto nos permitiría calcular los efectos de la temperatura en el espectro.

- Finalmente nos centramos en un problema particular, que es el de un átomo en contacto con el campo de radiación existente en un material de banda fotónica. Aparte de sus aplicaciones potenciales, este sistema es de amplio interés en sí mismo ya que por su carácter no-Markoviano presenta fenómenos físicos de gran interés. Desgranamos a continuación algunos de los resultados más importantes obtenidos en esta Parte,

  - Proponemos un nuevo modelo de función de correlación que describe el comportamiento a tiempos cortos de un modo más preciso que los modelos ya existentes. Con dicha función de correlación generamos el ruido correspondiente, que nos va a permitir emplear EES para el cálculo de los valores medios del sistema.
  - Con el esquema estocático, estudiamos algunos de los fenómenos físicos que han sido tratados en la literatura a través del uso de ecuaciones maestras: población residual del nivel excitado en el equilibrio, existencia de un estado enlazado átomo-fotón, e inversión de población en el equilibrio cuando el átomo es además sintonizado a un láser externo.

- Calculamos algunas funciones de correlación a dos tiempos de operadores del sistema. Dichas funciones son necesarias para computar el espectro de emisión atómico, lo cual conecta directamente con algunas de las perspectivas que el presente trabajo deja abiertas. Esto se explica con más detalle en la siguiente Sección.

18.7 PERSPECTIVAS

Las últimas dos Partes de esta tesis, concernientes a FCM y a sus aplicación a sistemas en contacto con materiales de banda fotónica, dejan abierta la posibilidad de computar el espectro de emisión y la estadística de fotones de dichos sistemas, siempre en el límite de acoplamiento débil.

Resulta especialmente interesante el estudio del espectro de emisión de un átomo con interacción de tipo no Markoviano, ya que éste ha de presentar una forma muy distinta del perfil Lorentziano típico de interacciones Markovianas. Puede ser también interesante a la hora de estudiar cómo dicho carácter Markoviano afecta al espectro de fluorescencia intermitente de un átomo de tres niveles immerso en un material de banda fotónica. Por otro lado, en el estudio de la estadística de fotones, resulta de particular interés determinar si también en el caso no-Markoviano existe el efecto de *anti-buching* que ha sido ampliamente estudiado en la literatura en sistemas Markovianos.

Dado que hemos derivado formalmente la ecuación de evolución de funciones de correlación a dos tiempos para sistemas en un entorno térmico, sería igualmente interesante aplicar dichas ecuaciones a un sistema cuántico abierto en particular. Resultaría de especial interés el cómputo de cantidades tales como el espectro de emisión, estudiando como éste se ve afectado por la temperatura. También sería posible derivar las ecuaciones que obedecen las funciones de correlación a N tiempos, ya que dicho cálculo no presenta ninguna diferencia cualitativa respecto al cálculo de la ecuación de funciones de correlación a dos tiempos.

Asímismo, aún no ha quedado aún resuelto en la literatura el problema de la interpretación de las trajectorias no-Markovianas como resultantes de un experimento de medida. En dichas medidas el estado del sistema se conoce indirectamente a través de medir el estado del entorno. El problema que presenta el caso no-Markoviano, es que al monitorizar el entorno, éste sufre una alteración de la que no se recupera instantáneamente, como ocurre en el caso Markoviano, lo cual afecta a las siguientes medidas. El tiempo durante el cuál el entorno se ve afectado por la interacción, en este caso con el aparato de medida, no es otro que el tiempo de memoria o tiempo de correlación. Nuestra propuesta supone considerar un conjunto de medidas sobre el sistema no-Markoviano separadas por un intervalo de tiempo escogido como $\Delta t > \tau_c$, lo cual permite que el entorno se recupere entre ellas. Suponiendo que el estado del entorno haya sido medido sobre una base de estados Bargmann, podemos expresar el estado después de la misma en función del propagador reducido del sistema que va desde el estado del baño medido, z_{i+1}, hasta el estado al que es projectado después, z_i. Resulta de especial interés en este esquema el conocimiento de la ecuación de evolución de propagadores que no partan del vacío, sino de un determinado estado z_{i+1}, ecuación que ha sido propuesta por primera vez a lo largo de esta tesis.

Finalmente, las ecuaciones de evolución derivadas en esta tesis podrían ser utilizadas para calcular la dinámica de muchos otros sistemas en los que existe interacción de tipo no-Markoviano, siempre y cuando éstos esten linealmente acoplados con su entorno. Queda abierta también la posibilidad de aplicar otras aproximaciones a la ecuación de evolución del propagador reducido, así como a la jerarquía de FCM.

References

1. I. de Vega, D. Alonso, P. Gaspard, and W.T. Strunz, J. Chem. Phys. **122** 1, (2005).
2. I. de Vega and D. Alonso, *Hierarchy of non-Markovian multiple time correlation functions*, La Laguna, preprint (2005).
3. D. Alonso and I. de Vega, Phys. Rev. Lett. **94**, 200403 (2005).
4. I. de Vega and D. Alonso, *Non-Markovian reduced propagator: Multiple-time correlation functions and master equations with general initial conditions*, La Laguna, preprint (2005).
5. I. de Vega, D. Alonso and P. Gaspard, Proceedings of SPIE, **5468**, 219 (2004).
6. I. de Vega, D. Alonso and P. Gaspard, Phys. Rev. A **71**, 023812 (2005).
7. N. G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 2nd. ed.,North Holland, Amsterdam (1992).
8. D. Alonso, A. Ruíz, and I. de Vega, Phys. Rev. E **66**, 066131 (2002).
9. D. Alonso, A. Ruíz, and I. de Vega, Physica D, **187**, 184 (2004).
10. E.M. Purcell, Phys. Rev. **69**, 681 (1946).
11. D. Kleppner, Phys. Rev. Lett. **47**, 233 (1981).
12. E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
13. S. John, Phys. Rev. Lett. **58**, 2486 (1987).
14. V. Weisskopf and E. P. Wigner, Z. Phys. **63**, 54 (1930).
15. G. Lüders, Ann. Phys. (Leipzig), **8**, 323 (1951); J. von-Neumann, *Mathematical Fundations of Quantum Mechanics*, Princenton University, Princenton, N.J. (1955).
16. L.D.Landau and E.M. Lifschitz, *Statistical Physics, Part I*, Pergamon Press, Oxford (1980).
17. L. Onsager, Phys. Rev. **37**, 405 (1931); **38**, 2265 (1931).

18. M. Lax, Phys. Rev. **129**, 2342 (1963).
19. M. Lax, Phys. Rev. **157**, 213 (1967).
20. A. O. Caldeira and A. J. Leggett, Physica A **121**, 587 (1983).
21. D.F. Walls and G.J. Milburn, *Quantum Optics*, Springer-Verlag, (1995).
22. U. Weiss *Quantum Dissipative Systems*, Series in Modern Condensed Matter Physics, vol. 10, World Scientific.
23. See for example: S. John and T. Quang, Phys. Rev. Lett. **74**, 3419 (1995); B. Garraway, Phys. Rev. A **55**, 2290 (1997); N. Vats and S. John, Phys. Rev. A bf 58, 4168 (1998).
24. S. Bay, P. Lambropoulos, and K. Mølmer, Phys. Rev. A **57**, 3065 (1998).
25. G.M. Nikolopoulos, S. Bay and P. Lambropoulos, Phys. Rev. A **60**, 5079 (1999).
26. M.W. Jack and J.J. Hope, Phys. Rev. A **63**, 5079 (2001).
27. S. John, and T. Quang, Phys. Rev. A **50**, 1764 (1994).
28. S. John, and T. Quang, Phys. Rev. Lett. **74**, 3419 (1995).
29. M. Lewenstein, J. Zakrzewski, and T. W. Mossberg, Phys. Rev. A **38**, 808 (1988).
30. J.J. Hope, Phys. Rev. A, **55**, 2531 (1997).
31. J.J. Hope, G.M. Moy, M.J. Collet, and C.M. Savage, Phys. Rev. A, **61**, 023603 (2000).
32. H.P. Breuer, D. Faller, B. Kappler, and F. Petruccione, Europhys. Lett. **54**, 14 (2001).
33. S. Chakravarty and A.J.Leggett, Phys. Rev. Lett. **52**, 5 (1984).
34. A.J.Leggett, S. Chakravarty, A. T. Dorsey, Matthew P.A. Fisher, A. Garg and W. Zwerger. Rev. Mod. Phys. **59**,1 (1997).
35. P. Gaspard and M. Nagaoka, J. Chem. Phys.**13**, 5676 (1999).
36. G. Lindblad, Commun. Math. Phys. **48**, 119(1976); G, V. Gorini, A. Kossakowski and ECG Sudarshan, J. Math. Phys. 17, 821 (1976).
37. P. Gaspard, and M. Nagaoka, J. Chem. Phys. **111**, 5668 (1999).
38. H.P. Breuer and F. Petruccione, *The theory of open quantum systems*, Oxford University Press, (2002).
39. L. Diósi and W. T. Strunz, Phys. Lett.A **235**, 569 (1997).
40. L. Diósi, N. Gisin and W. T. Strunz, Phys. Rev. A **58**, 1699 (1998).
41. W. T. Strunz, Chem. Phys. **268**, 237 (2001).
42. Marian Florescu and S. John, Phys. Rev. A. **64**, 33801 (2001).
43. M. O. Scully and M. Suhail Zubairy, *Quantum Optics*, Cambridge University Press, (1997).
44. A. O. Barut, and J.P. Dowling, Phys. Rev. A **36**, 649 (1987).
45. C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics, Vol II*, Wiley-Interscience (1977).
46. M. Woldeyohannes and S. John, Journal of Optics B: Quantum and Semiclassical Optics **5**, R43-R82 (2003).
47. V. Bargmann, Commun. Pure and Appli. Math. **14**, 187 (1961); Proc. Natl. Acad. Sci. U.S. **48**, 199 (1962).

48. R.J. Glauber, Phys. Rev. **131**, 2766 (1963).
49. A. A. Budini, Phys. Rev. A **63**, 012106 (2000).
50. C. Cohen-Yannoudji, J.Dupont-Roc and G. Grynberg, *Atom-Photon Interactions. Basic Processes and Applications*, Willey Interscience (1992).
51. C. W. Gardiner and P. Zoller, *Quantum Noise*, 2nd ed. (Springer, Berlin), (2000).
52. H.J.Carmichael, *Statistical Methods in Quantum optics 1. Master equations and Fokker Plank equations*, Springer-Verlag (1999).
53. H.J. Carmichael, *Statistical Methods in Quantum Optics 1. Master Equations and Fokker-Planck Equations*, Springer-Verlag, (2002).
54. T. Yu, L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **90**, 91 (1999).
55. Walter T. Strunz and Ting Yu, Phys. Rev. A **69**, 052115 (1004).
56. N. Gisin, J. of Mod. Opt. **40**, 2313 (1993).
57. Dirk G. Sondermann, J. of Mod. Opt. **42**, 1659 (1995).
58. Tood A. Brun and Nicolas Gisin, J. of Mod. Opt. **43**, 2289 (1996).
59. Heinz-Peter Breuer, Bernd Kappler and Francesco Petruccione, arXiv:quant-ph/9807082 (1998).
60. Heinz-Peter Breuer, Eur. Phys. Jour. D **29**, 106.118 (2004).
61. Heinz-Peter Breuer,Phys. Rev. B **70**, 045323 (2004).
62. P. Zoller, M. Marte, and D.F. Walls, Phys. Rev. A **35**, 198 (1987).
63. G.C. Hegerfeldt, and T.S. Wilser, *Proceedings of the II International Wigner Symposium*, edited by H.D. Doebner, W. Sherer, and F. Schroeck, World Scientific Singapore, P. 104 (1991).
64. C. W. Gardiner, A. S. Parkins and P. Zoller, Phys. Rev. A **46**, 4363 (1992).
65. J. Dalibard, Y. Castin and K. Mølmer, Phys. Rev. Lett. **68**, 580 (1992).
66. K. Mølmer, Y. Castin, and J. Dalibard, J. Opt. Soc. Am. B **10**, 524 (1993).
67. M. B. Plenio and P. L. Knight, Rev. Mod. Phys **70**,101 (1998).
68. N. Gisin and I. C. Percival, J. Phys. A **25**, 5677 (1992).
69. N. Gisin and I. C. Percival, J. Phys. A **26**, 2245 (1993).
70. J. D. Cresser, Laser Phys. **10**, 1, (2000).
71. W.T. Strunz, L. Diósi, and N. Gisin, Phys. Rev. Lett. **82**, 1801 (1999).
72. A. Einstein, Phys. Zeits. **18**, 121 (1917).
73. W. Pauli, Festschrift zum 60 Geburstag A. Sommerfeld S.30. (Leipzig, Hirzel 1928).
74. C. Cohen-Tannoudji, B. Diu, F. Laloë. *Quantum Mechanics Volume I*, Willey-Interscience (1977).
75. A. G. Redfield, IBM J. Res. Dev. **1**, 19 (1957); Adv. Magn. Reson. **1**, 1 (1965).
76. Heinz-Peter Breuer, Bernd Kappler and Francesco Petruccione, Phys. Rev. A **59**, (1999).
77. . P. Pechukas, Phys. Rev. Lett. **73**, 1060 (1994).
78. A. Suárez, R. Silvey, and I. Oppenheim, J. Chem. Phys. **97**, 5101 (1992).
79. S. Nakajima, Prog. Theor. Phys. **20**, 948 (1958).
80. R. Zwanzig, J. Chem. Phys **33**, 1338 (1960).

81. Heinz-Peter Breuer, Phys. Rev. A **70**, 012106 (2004).
82. P. Pearle, Phys. Rev. D, **13**, 857 (1976).
83. N. Gisin, Phys. Rev. Lett. **52**, 1657 (1984).
84. P.Pearle, Phys. Rev. A **39**, 2277(1989).
85. G.C. Ghirardi, A. Rimini, and T. Weber, Phys. Rev. D **34**, 470 (1986).
86. G.C. Ghirardi, P. Pearle, A. Rimini, Phys. Rev. A **42**, 78 (1990).
87. A. Bassi, G.C. Ghirardi, Phys. Reports **389**, 257 (2003).
88. N. Gisin, I. C. Percival, J. Phys. A: Math. Gen **26**, 2233-2243 (1993).
89. V. P. Belavkin, Phys. Lett. A **140**, 355 (1989).
90. V. P. Belavkin, J. Math. Phys. **31**, 2930 (1990).
91. V. P. Belavkin, and P. Staszewski, Phys. Rev. A. **45**, 1347 (1992).
92. P. Goetsch, R. Graham, and F. Haake, Phys. Rev. A **51**, 136 (1995).
93. H.M. Wiseman and G.J. Milburn, Phys. Rev. A **47**, 642 (1993).
94. J. Gambetta and H.M. Wiseman, Phys. Rev. A, ,**66**, 012108 (2003).
95. A. Imamoglu, Phys. Lett. A **224**, 3650 (1994).
96. A. Imamoglu, Phys. Rev. A **50**, 3650 (1994).
97. B.M. Garraway, Phys. Rev. A **55**, 2290 (1997).
98. S. Bay, P. Lambropoulos, and K. Mølmer, Phys. Rev. Lett. **75**, 2654 (1997).
99. M.W. Jack, M.J. Collet, and D.F. Walls, Phys. Rev. A **59**, 2306, (1999).
100. M. W. Jack and M. J. Collet, Phys. Rev. A **61**, 06216 (2000).
101. E. B. Davies, *Quantum Theory Of Open Systems*, Academic, New York (1976).
102. K. Kraus, *States, Effects, and Operators: Fundamental Notions of Quantum Theory*, Springer, (1983).
103. H.M. Wiseman, Quantum Semiclass. Opt. **8**, 205-222 (1996).
104. D.Gatarek and N.Gisin, J.Math.Phys. **32**, 2152 (1991).
105. R. P. Feynman and F. L. Vernon, Ann Phys. (N.Y) **24**, 118 (1963).
106. See, for example, N.W. Ashcroft and N.D. Mermin, *Solid State Physics* (1976).
107. H.J. Carmichael, and D.F. Walls, J. Phys. B **9**, L43 (1976); J. Phys. B **9**, 1199 (1976).
108. H.J. Kimble, M. Dagenais, L. Mandel, Phys. Rev. Lett. **39**, 691
109. See for example: S. John and T. Quang, Phys. Rev. A **50**, 1756 (1994); S. Bay, P. Lambropoulos and K. Mølmer, Phys. Rev. Lett. **79**, 2654 (1997); M. W. Jack and J. J. Hope, Phys. Rev. A **63**, 043803 (2001); G. M. Nikolopoulos and P. Lambropoulos, Phys. Rev. A **61**, 053812 (2000). (1977); Phys. Rev. A **18**, 201 (1978).
110. Justiniano Casas, *Optica*, Librería General, Zaragoza (1994) .
111. S. John, Phys. Rev. Lett. **53**, 2169 (1984).
112. E. Yablonovitch, T.J Gmitter, and K.M. Leung, Phys.Rev.Lett. **65**, 3152 (1990).
113. S. John and T. Quang, Phys. Rev. A**50**, 1764 (1994); A. Kaufman, G.Jurizki and B. Sherman, J. Mod. Opt. **41**,353 (1994); Y. Yang and S. Y Zhu, *ibid***62**, 013805 (2000).

114. S. John and T. Quang, Phys. Rev. Lett. **78**, 1888 (1997).
115. Gyeong-il Kweon and N.M.Lawandy, Optics Communications **118**, 388 (1995).
116. S. John and T. Quang, Phys. Rev. Lett **74**, 3419 (1995).
117. S. John and J. Wang, Phys. Rev. Lett **64**, 2418 (1990).
118. S. John and J. Wang, Phys. Rev. B **43**, 12772 (1991).
119. S. John, Phys. Today **44**, 32 (1991).
120. A. Blanco et. al., Nature (London) **405**, 437 (2000).
121. Gyeong-il Kweon and N.M. Lawandy, Opt. Comm **118**, 388-411 (1995).
122. K. Busch, C.R. Physique **3**, 53-66 (2002).
123. K.M.Ho, C.J.Chan and C.M. Soukoulis, Phys.Rev.Lett. **65**,3152 (1990).
124. Lin S.Y. et.al. Nature **394**, 251 (1998).
125. H.Minguez et. al. Phys.Rev.B **59**, 1563 (1999).
126. A. Chutinan and S. Noda, Phys.Rev.B **57**, 2006 (1997).
127. L. Diósi, Phys. Lett. A **132**,233 (1988).
128. L. Diósi, J. Phys. A **21**, 233 (1988).
129. J. J. Hope, Phys. Rev. A **55**, 2531 (1997); J. J. Hope, G. M. Moy, M. J. Collet and C. M. Savage, Phys Rev. A **61**, 023603 (2000).
130. W. T. Strunz, Phys. Lett. A. **224**, 25 (1996).
131. C. W. Gardiner and P. Zoller, *Quantum Noise*, 2nd ed. (Springer, Berlin), (2000)
132. P.R. Holland *The Quantum Theory of Motion. An Account of the Broglie-Bohm Causal Interpretation of Quantum Mechanics*, Cambridge Univ. Press, (1993).
133. R. Zwanzig, *Nonequilibrium Statistical Mechanics*, Oxford University Press (2001).
134. N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, North Holland (1981).
135. H.M. Wiseman, Quantum Semiclass. Opt. **8**, 205-222 (1996).
136. B. Misra and E.C.G. Sudarshan, J. Math. Phys, **18**, 756 (1977).
137. R. Reibold, J. Phys. A **26**, 179 (1993).
138. W. T. Strunz.Unpublished.
139. J. Gambetta, and H. M. Wiseman, Phis. Rev. A, **68**, 062104 (2003).
140. M.V. Berry, J. Phys. A **10**, 2083 (1977); A. Voros, Ann. Inst. Henri Poincaré, Sect. A **24**, 31 (1976); M. Shapiro, J. Ronkin and P. Brumer, Chem. Phys. Lett. **148**, 177 (1988).
141. M. Srednicki, Phys. Rev. E **50**, 888 (1994); **54**, 954 (1996); S. Hortikan and M. Srednicki, Phys. Rev. Lett. **80**, 1646 (1998). .
142. G.N. Watson, *Theory of Bessel Functions*, 2nd ed. (Cambridge University Press, Cambridge, 1952)
143. C. W. Gardiner *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences*, Springer-Verlag (1990).
144. Nipun Vats, S. John and Kurt Busch, Phys. Rev. A **65**, 43808 (2002).
145. H.G. Dehmelt, Bull. Am. Phys. Soc. **20**, 60 (1975).

146. H.G. Dehmelt, IEEE Trans. Instrum. Meas. IM-31, 83 (1982).
147. R.J. Cook, and H.J. Kimble, Phys. Rev. Lett. **54**, 1023 (1985).
148. H.J. Kimble, R.J. Cook, and A.L. Wells, Phys. Rev. A **34**, 3190 (1986).
149. G.S. Argawall, S.V. Lawarde, and R.D'Souza, Phys. Rev. A **37**, 444 (1988).
150. G.C. Hegerfeldt, and M.B. Plenio, Phys. Rev. A **52**, 3333 (1995).