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AN OPEN QUANTUM SYSTEM COUPLED TO AN OPEN ENVIRONMENT

Andreu Anglés Castillo

Tutor (1): Armando Pérez (UV i IFIC)
Tutora (2): Inés de Vega (LMU)
Tutora (3): Mari Carmen Bañuls (MPQ)

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Abstract

The purpose of the present work is the study of open quantum systems, i.e., quantum systems surrounded by an environment with which they interact. We present the basic models that describe this situation, and show a method to study the evolution. We apply this evolution to various kinds of environments, and consider the novel interesting case of a system coupled to two environments in a hierarchical way.

1 Introduction

We are going to focus our study on Open Quantum Systems (OQS). An OQS is a quantum-mechanical system which interacts with an external, usually much larger, quantum system: the environment [1, 2]. In practice, each quantum system should be considered as an OQS to some extent as full isolation in the quantum world is impracticable, therefore this field of study is applicable almost to any quantum discipline. The most important ones are quantum optics, quantum computing and quantum information, measurement theory, quantum thermodynamics, as well as quantum statistics. In most situations the environment may have a large number of degrees of freedom, even infinitely many, which makes the problem hard to tackle with. Even when the study of the full system (OQS and environment) is possible, it requires a lot of computational power. That's why some approximate methods have to be developed to account for the environment, but finally focus on the sole evolution of the OQS. The theory of OQS seeks the understanding of the dynamics of the system.

The principal effects that open quantum systems undergo are quantum dissipation, which is the transfer of energy from the OQS onto the environment, and quantum decoherence. This last effect has a fundamental role in understanding the quantum-to-classical transition [3], that is, how is that the world is described by quantum mechanics, yet no quantum mechanical effect is observed at macroscopic scales. Decoherence plays the role of washing out quantum mechanical effects, namely, the loss of quantum entanglement or, in other words, quantum correlations. The effect that the environment induces onto the OQS has been extensively studied for very different environments, depending on its temperature, the number of degrees of freedom, its coupling strength to the OQS, its density of states, etc.

The standard scenario considered is that in which the open system is directly coupled to a single environment, which is assumed to be initially in an equilibrium state. Both system and environment are assumed to conform a closed system that may evolve according to a highly complex but still unitary dynamics. This idea has been extended to the case where the open system is coupled to two or more environments at different temperatures, as it occurs in the context of quantum thermodynamics. However, the case where the open system is coupled to an environment, which in turn is coupled to a second one that acts as a reservoir for it, has not been studied in the literature, to the best of our knowledge. This situation can represent, for instance, atoms coupled to the electromagnetic field within a waveguide that includes vibrational modes, i.e. in the presence of an optomechanical coupling. In this case a new time scale comes into play, which is that of the relaxation of the first environment when coupled to the second one. During such relaxation time the first environment is taken away from its equilibrium initial state, and therefore its fluctuations are no longer the equilibrium ones. The interesting aspect is that, according the the theory of open system which we will extend in this work, such environment

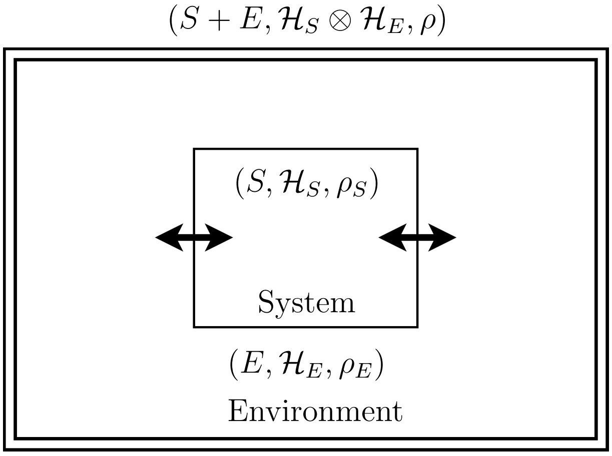


Figure 1: Schematic picture of an open quantum system. The total system $S+E$ is isollated, and the central OQS S interacts with the environment E.

fluctuations will also determine the open system dynamics, leading to dissipation and decoherence processes that are crucially affected by the presence of the second environment. In this work we present the theoretical framework and explore some effects that this new paradigm can have in the theory of OQS.

The common approach in the study of OQS is to describe the quantum states of the total system using the density matrix formalism to consider pure states, as well as ensembles of pure states (mixed states). The density matrix is a positive trace class operator on the Hilbert space of the system it describes. A trace class operator is an operator in a Hilbert space $\mathcal{H}$ for which a trace may be defined, such that it is finite and independent of the choice of basis. The following properties characterize the density matrix operator:

- **Hermiticity** $\rho = \rho^\dagger$ This property ensures that the eigenvalues of the density matrix are all real and that there exists an orthogonal basis to express this matrix in the diagonal form.
- **Normalization** Density operators represent state probabilities, therefore, some normalization is required, namely, $\mathrm{Tr}\rho = 1$. Following from the independence of the trace and the previous property, the trace of any density operator is $\mathrm{Tr}\rho = \sum_i \lambda_i$, where λ_i are the eigenvalues of ρ.
- **Positive semi-defined** $\rho \geq 0$ An operator is positive semi-defined iff $\langle n|\rho|n\rangle \geq 0$ for any $|n\rangle \in \mathcal{H}$, which is equivalent to say that each eigenvalue of ρ is greater than or equal to 0. This property ensures that there are not negative probabilities.
- **Expectation values** are calculated as follows, $\langle A\rangle = \mathrm{Tr}\{\rho A\}$.

The Hilbert space of the total system is the tensor product of the individual Hilbert spaces, i.e., $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. The theory of OQS describes the state of the system and not that of the environment. This implies to put aside the environment state via partial tracing the total density matrix with respect to the environment. That is $\rho_S = \mathrm{Tr}_E\{\rho\}$, where $\rho_S \in \mathcal{H}_S$ and $\rho \in \mathcal{H}$. The partial trace is defined as $\mathrm{Tr}_E\{\rho\} = \sum_n (\mathbb{1}_S \otimes \langle n|)\rho(\mathbb{1}_S \otimes |n\rangle)$, where $\mathbb{1}_S$ is the identity operator in the Hilbert space of the OQS and $\{|n\rangle\}$ forms an orthonormal basis in $\mathcal{H}_E$. A schematic diagram of this situation is shown in Fig. 1.

This work is aimed on the study of the dynamics of the reduced density matrix of the system for different environments. To do so, we will introduce some elementary models to describe the evolution of OQS in section 2. In section 3 we introduce a function that encodes the action of the environment, and present a model that is commonly used. We introduce some basic concepts about the evolution of the reduced density matrix in section 4, where we will introduce the concept of Markovianity and the canonical master equation to describe a process of this kind. We also present the concept of non-Markovianity, its physical implications and a quantitative expression. In section 5 we will derive a master equation perturbatively. This master equation will be used for a variety of setups: the Weisskopf-Wigner theory in section 6, a pure dephasing mechanism in section 7, a thermal bath in section 8, and a thermal bath that is in turn coupled to another thermal bath in section 9.

2 OQS Models

There are many canonical models to describe OQS at low energies. We will consider only environments formed by harmonic oscillators, but there are models which deal with spin environments as well. These canonical models are formed by a central OQS linearly coupled to the environment. See Fig. 1 for a schematic diagram of this situation. The Hamiltonian for these canonical models have the following structure.

$$H = H_0 + H_I \ , \tag{1}$$

where H_0 is the free Hamiltonian of both the system and the environment, and H_I is the interaction Hamiltonian. The free Hamiltonian is composed by 2 terms, describing the free evolution of each system

$$H_0 = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E \ , \tag{2}$$

where H_S acts on $\mathcal{H}_S$ and H_E on $\mathcal{H}_E$ and $\mathbb{1}$ is the identity operator of each Hilbert space. We will use the shorthand notation $H_0 = H_S + H_E$, where it is understood to which Hilbert space each Hamiltonian belongs, that is we drop the identity operator whenever possible. We may also drop the tensor product symbol in future sections, where multiplication between operators living in different Hilbert spaces is understood to be of this nature. The interaction Hamiltonian acts on to the total Hilbert space as it describes the interaction between the system and the environment. The most general form that the interaction Hamiltonian can have that preserves the hermiticity property is [4]:

$$H_I = \sum_i (L_i \otimes B_i^\dagger + L_i^\dagger \otimes B_i) \ , \tag{3}$$

where L_i are operators acting on $\mathcal{H}_S$ and B_i on $\mathcal{H}_E$. We now present two of the most used models of OQS.

2.1 Spin-Boson model

The Spin-Boson model describes a spin-$\frac{1}{2}$ particle coupled to a environment composed of harmonic oscillators [1, 2, 5]. This model is of extreme importance in fields that deal with 2 level systems, or even with systems that have more degrees, but some of them can be truncated, in the low energy range, to present effectively two possible states. The free Hamiltonian for such a system is

$$H_0 = \frac{1}{2}\omega_0 \sigma_z + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda \ , \tag{4}$$

where natural units have been used ($\hbar = 1$), ω_0 is the energy separation of the 2 level system, $a_\lambda^\dagger$ and a_λ are the creation and annihilation operators of the λ oscillator with frequency ω_λ and any σ_X represents a Pauli matrix. Note that the vacuum energy of the harmonic oscillators of the environment has not been considered, as it only accounts for a constant shift in the energy. It is common to add a term of the form $\frac{1}{2}\Delta_0\sigma_x$ which represents the tunneling between the two levels of the spin-$\frac{1}{2}$ system [6]. The interaction Hamiltonian has the form

$$H_I = \sigma_x \sum_\lambda (g_\lambda^* a_\lambda^\dagger + g_\lambda a_\lambda) = \sigma_x \left(B^\dagger + B\right) \ , \tag{5}$$

where we defined $B = \sum_\lambda g_\lambda a_\lambda$, g_λ is the coupling strength between the spin and the λ oscillator, and σ_x can be decomposed as raising and lowering operators on the 2 level system as $\sigma_x = \sigma_+ + \sigma_-$, so that $\sigma_+ |-\rangle = |+\rangle$ and $\sigma_- |+\rangle = |-\rangle$, with $|+\rangle$ and $|-\rangle$ representing the upper and lower level of the OQS, respectively. It is often usual to simplify this Hamiltonian by assuming the rotating wave approximation (RWA). If we express the Hamiltonian (5) in the interaction picture, where the operators $\sigma_\pm$ and a_λ take the form

$$\hat{\sigma}_\pm(t) = \sigma_\pm e^{\pm i\omega_0 t} , \tag{6}$$

and

$$\hat{a}_\lambda(t) = a_\lambda e^{-i\omega_\lambda t} , \tag{7}$$

we get

$$\hat{H}_I(t) = \sum_\lambda \left(g_\lambda \sigma_+ a_\lambda e^{i(\omega_0-\omega_\lambda)t} + g_\lambda^* \sigma_- a_\lambda^\dagger e^{-i(\omega_0-\omega_\lambda)t} + g_\lambda^* \sigma_+ a_\lambda^\dagger e^{i(\omega_0+\omega_\lambda)t} + g_\lambda \sigma_- a_\lambda e^{-i(\omega_0+\omega_\lambda)t} \right) . \tag{8}$$

The RWA consists in keeping only the resonant terms, that is the terms that rotate with frequencies $|\omega_0 - \omega_\lambda|$. In this approximation the terms that do not conserve energy are discarded, i.e., those terms that correspond to a simultaneous excitation of the 2 level system and the creation of an energy quantum in the bosonic field, or the decay of the exited state and the annihilation of a boson. Within this approximation the interaction Hamiltonian becomes

$$H_I = \sum_\lambda \left(g_\lambda^* \sigma_- a_\lambda^\dagger + g_\lambda \sigma_+ a_\lambda \right) . \tag{9}$$

The dynamics of this model is extremely rich, and is the main point of this work, where we study the evolution of a 2 level system coupled to a continuum of harmonic oscillators which are in thermal equilibrium. The usual example of a system described by this model is a two-level atom interacting with the vacuum quantized modes of an optical cavity. This particular situation is described by the so-called Jaynes-Cummings model (JCM) [7], which is exactly solvable under the RWA. This model will be of particular interest to check whether the approach we take in the following sections to describe the OQS dynamics reproduces the exact dynamics of the JCM.

2.2 Caldeira-Leggett model

The Caldeira-Leggett model was introduced in 1983 [8, 9] to describe the effect of dissipation of a particle coupled to an environment. It describes a particle with mass m and coordinate x under the effect of a potential $V(x)$, coupled to an environment of harmonic oscillators. The free Hamiltonian of the particle plus the environment is described by

$$H_0 = \frac{1}{2m}p^2 + V(x) + \sum_n \left(\frac{1}{2m_n} p_n^2 + \frac{1}{2} m_n \omega_n x_n^2 \right) , \tag{10}$$

where p is the momentum of the particle and p_n, m_n and x_n are the momentum, mass and position of the n-th oscillator of the environment, respectively. The interaction between the particle and the environment is supposed to be of the form

$$H_I = -x \sum_n k_n x_n , \tag{11}$$

with k_n the coupling strength to the n-th oscillator. This interaction will yield a renormalization of the potential of the particle, so that a counter term is added to the total Hamiltonian of the system, which acts only on the Hilbert space of the OQS. This model has been of great importance, as it describes the quantum Brownian motion and allows a description of classical dissipation from a quantum point of view when taking the classical limit.

3 Characterizing the environment

For environments described by a discrete set of harmonic oscillators, the interaction is characterized by the spectral density, defined as

$$J(\omega) = \pi \sum_{\lambda} g_{\lambda}^{2} \delta(\omega - \omega_{\lambda}) \ , \tag{12}$$

where g_λ are the couplings between the OQS and the λ-th oscillator of the environment. This function encodes the effect that the environment has onto the OQS. Such action can also be characterized by the environment correlation function, which for environments that are at zero temperature, becomes a partial Fourier transform of $J(\omega)$

$$\alpha(t) = \int_{0}^{\infty} d\omega J(\omega) e^{-i\omega t} \ . \tag{13}$$

These correlation functions will be re-defined when deriving a master equation for the dynamics of the reduced density matrix of the OQS, and will play the role of past evolution of the system, from which memory effects may take place. These effects will be further discussed in the following section. These correlations will take different forms depending on the properties of the environment we are dealing with. For instance, for thermal environments, these functions will be modulated by the thermal distribution function. In the limit of a large number of oscillators, a continuum representation of the couplings can be performed $g_\lambda \to g(\omega)$. If we know the dispersion relation, the spectral density can be written in the continuum as

$$J(\omega) = g^{2}(h(\omega)) D_{DOS}(\omega) \ , \tag{14}$$

where $h(\omega) = k$ is the inverse dispersion relation, and $D_{DOS}(\omega) = |\partial\omega(k)/\partial k|^{-1}$ is the bosonic density of states (DOS). Depending on the nature of the environment, different nomenclature is used to refer to it. We will follow the standard nomenclature found in the literature. We will use the word *environment* to refer to the more general subsystem that is coupled to the OQS, assumed to be much larger than the OQS. A *reservoir* is an environment with a continuum spectrum and the expression *bath* will be reserved to refer to reservoirs that are in a thermal equilibrium state.

There exist two ways to obtain these spectral density functions. On the one hand, the continuum version in Eq. (14) allows for a microscopic derivation of the spectral density function if knowledge about the interaction is available, that is the expression for the coupling constants g_λ and the dispersion relation $\omega(k)$. This derivation is possible, for example, for atoms interacting with electromagnetic fields, where the dispersion relation relation in vacuum is well known, as well as the coupling constants. On the other hand, if no microscopic description of the environment is available, a phenomenological modelling of the spectral density is used. The most used model is the one by Caldeira and Leggett [8],

$$J(\omega) = g\omega^{s} e^{-\omega/\omega_c} \ , \tag{15}$$

where the parameter g describes the coupling strength between the system and the environment. The exponential factor provides a smooth regularization of the spectral density function modulated by a cut-off frequency ω_c. This cut-off frequency has to be properly chosen in accordance to other scales of the problem. The parameter ω_c describes the bandwidth of the reservoir, a higher ω_c describes a reservoir with more modes. A Lorenz-Drude regularization could also be used, as in the case of the Breit-Wigner distribution function. Depending on the parameter s, many different types of reservoirs can be described. Environments with $0 < s < 1$ are called sub-ohmic, and those with $s = 1$ and $s > 1$ are considered as ohmic and super-ohmic, respectively. This spectral density is widely used for its versality, for instance, for $s = 1$ represents the vacuum radiation, and for $s = 1/2$ isotropic photonic crystalls. It can also model a phonon environment where the parameter s can have various values depending on the dimension and symmetry properties of the field [5].

4 Evolution, Dynamical Maps, Master Equations and Markovianity

The evolution of a quantum state is given by the Schrödinger equation, the equivalent for density matrices is often referred to as the Liouville-von Neumann equation and has the following expression

$$\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)] \ , \tag{16}$$

where $H(t)$ is the Hamiltonian of the total system. The solution to this equation is

$$\rho(t) = U(t, t_0)\rho(t_o)U^\dagger(t, t_0) \ , \tag{17}$$

where $U(t, t_0)$ is the unitary time evolution operator which, for time independent Hamiltonians, has the usual expression

$$U(t, t_0) = e^{-iH(t-t_0)} \ . \tag{18}$$

When dealing with Hamiltonians of the form (1), where H_0 is time independent and H_I can be time dependent, it is usual to switch to the interaction picture. The density matrix in the interaction picture is defined as

$$\hat{\rho}(t) = U_0^\dagger(t, t_0)\rho(t)U_0(t, t_0) \ , \tag{19}$$

where $U_0(t, t_0) = \exp[-iH_0(t - t_0)]$. With this definition it is straightforward to see, by direct differentiation and substitution of (16), that the evolution equation for the interaction picture density matrix operator is

$$\frac{d}{dt}\hat{\rho}(t) = -i[V_t^0 H_I(t), \hat{\rho}(t)] \ , \tag{20}$$

where we defined $V_t^0 H_I(t) = U_0^\dagger(t, t_0)H_I(t)U_0(t, t_0)$, which is the interaction Hamiltonian in the interaction picture. An equivalent equation, obtained by formal integration of (20), is

$$\hat{\rho}(t) = \hat{\rho}(t_0) - i\int_{t_0}^{t} d\tau [V_\tau^0 H_I(\tau), \hat{\rho}(\tau)] \ , \tag{21}$$

which will be useful in deriving a perturbation approach for the dynamics of the reduced density matrix of the system in the following section. If we now want to extract the evolution of the OQS we can take the partial trace of equation (17)

$$\rho_S(t) = \mathrm{Tr}_E\rho(t) = \mathrm{Tr}_E\{U(t, t_0)\rho(t_o)U^\dagger(t, t_0)\} \ , \tag{22}$$

which, in terms of the differential Eq. (16), is equivalent to

$$\frac{d}{dt}\rho_S(t) = -i\mathrm{Tr}_E[H(t), \rho(t)] \ . \tag{23}$$

A common assumption to take is that the state of the OQS and the environment are initially uncorrelated, i.e., $\rho(0) = \rho_S(0) \otimes \rho_E(0)$, where we set $t_0 = 0$ for simplicity. Now $\mathrm{Tr}_E\rho(0) = \rho_S(0)$ and the evolution of $\rho_S(t)$ is given by (22). So the transformation $\phi(t)$ that maps

$$\rho_S(0) \mapsto \rho_S(t) = \phi(t)\rho_S(0) = \mathrm{Tr}_E\{U(t, 0)\rho(0)U^\dagger(t, 0)\} \ , \tag{24}$$

$$\begin{tikzcd}
\rho(0) = \rho_S(0) \otimes \rho_E \arrow[r, "\text{unitary evolution}"] \arrow[d, "\mathrm{Tr}_E"'] & \rho(t) = U(t,0)[\rho_S(0) \otimes \rho_E]U^\dagger(t,0) \arrow[d, "\mathrm{Tr}_E"] \\
\rho_S(0) \arrow[r, "\text{dynamical map}"] & \rho_S(t) = \phi(t)\rho_S(0)
\end{tikzcd}$$

Figure 2: A diagram showing the action of the dynamical map $\phi(t)$. It is possible to evolve the whole system and partial trace the environment to obtain the dynamics of the OQS, or the evolution of the OQS can be described by the dynamical map.

is called a quantum dynamical map. A schematic diagram of this procedure is shown in Fig. 2. A dynamical map must preserve the properties of the density matrix introduced in the first section, that is, it must be a completely positive trace preserving (CPT) map. A map is positive if it keeps the final density matrix positive. The condition of complete positivity is a bit tricky. Imagine you have an auxiliary Hilbert space $\tilde{\mathcal{H}}$ which has no interaction at all with the OQS nor to the environment, then the map is completely positive iff $(\phi(t) \otimes \mathbb{1})\tilde{\rho} \geq 0$ with $\tilde{\rho} \in \mathcal{H}_S \otimes \tilde{\mathcal{H}}$, for any $\tilde{\mathcal{H}}$. The one parameter family $\{\phi(t) | t \geq 0\}$ describes the future time evolution of the open system and $\phi(0)$ is the identity map. Note that only positive times are considered. This evolution can also be expressed in the following way

$$\rho_S(t) = \mathrm{Tr}_E\{U(t,0)(\rho_S(0) \otimes \rho_E(0))U^\dagger(t,0)\} = \sum_{i,j} p_i \langle j|U(t,0)|i\rangle \, \rho_S(0) \, \langle i|U^\dagger(t,0)|j\rangle \ , \tag{25}$$

where the states $|j\rangle$ form an orthonormal basis in $\mathcal{H}_E$ and the environment state was decomposed in its diagonal form $\rho_E(0) = \sum_i p_i |i\rangle \langle i|$, where $\sum_i p_i = 1$. Defining the Kraus operators as $K_{ij} = \sqrt{p_i} \langle j|U(t,0)|i\rangle$ we can write

$$\rho_S(t) = \sum_{i,j} K_{ij}(t)\rho_S(0)K_{ij}^\dagger(t) \ , \tag{26}$$

where $\sum_{i,j} K_{ij}(t)K_{ij}^\dagger(t) = \mathbb{1}_S$.

There is a special sub-class of maps which obey the following additional property

$$\phi(t_1)\phi(t_2) = \phi(t_1 + t_2), \quad t_1, t_2 \geq 0 \ , \tag{27}$$

which is called the semigroup property. Maps obeying this property form a semigroup as the map cannot have negative arguments, therefore, no inverse exists. This property is also referred to as the divisibility property. Maps obeying this property are called Markovian, that is, the evolution only depends of the previous instant of time and not on the whole history of the system evolution. For maps with property (27) there exist a linear operator $\mathcal{L}$, the generator of the semigroup, which allows to express them in the exponential form

$$\phi(t) = e^{\mathcal{L}t} \ . \tag{28}$$

From this fact and definition (24) a first-order differential equation for the reduced density matrix of the system can be readily written as

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t) \ , \tag{29}$$

which represents what is called a Markovian master equation for the dynamics of the reduced matrix for the system, also called Lindblad master equation. It can formally be shown [10, 11, 1] that the most general form of this generator, assuring that $\phi(t)$ is CPT and divisible, is

$$\mathcal{L}\rho_S(t) = -i[H, \rho_s(t)] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S(t) A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S(t) - \frac{1}{2} \rho_S(t) A_k^\dagger A_k \right) , \tag{30}$$

where N is the dimension of the Hilbert space $\mathcal{H}_S$. The first term of the generator represents the unitary part of the evolution of system S, although H cannot directly be identified with the free Hamiltonian of the open system, because it may contain interaction terms with the environment that cause a shift in the energies of the open system. The second term is called the dissipator, and the operators A_k, called Lindblad operators, describe the decay modes of the system, where the γ_k are their corresponding decay rates. These decay rates have to be positive in order to keep the map $\phi(t)$ completely positive and divisible.

The *memoryless* behavior that Markovian maps present describes well many physical systems under certain assumptions. The assumption that a physical system has to obey in order to be well described by a Markovian evolution is that the relaxation time of the OQS is much larger than the one of the environment. In this scenario, any change that the OQS induces into the environment will rapidly be washed out and the environment will recover its initial state quasi instantaneously. This behavior of the system is described by a correlation function of the environment that approximates a delta function $\alpha(t-\tau) \sim \delta(t-\tau)$, whereas the changes induced onto the OQS do not decay so fast. This allows to evolve the OQS from its current state independently of the past evolution, as OQS and environment stay uncorrelated along the whole process when the evolution is Markovian.

When such assumptions about the environment cannot be made, the previous dynamical semigroup is broken and memory effects take part in the evolution. Processes in which the evolution cannot be expressed as a dynamical semigroup are referred to as non-Markovian, and the physical interpretation of what is happening is that there is a backflow of information from the environment into the OQS. That is, Markovian processes reduce the distinguishability between states of the OQS during the whole evolution, while, in the non-Markovian case, the distinguishability can be recovered. Even thought the Markov approximation is not valid for some physical situations, as long as the dynamical map is invertible and differentiable, there exist a time local master equation for the reduced density matrix operators. This is shown in [11] by computing the derivative of Eq. (26) and decomposing the system operators in a basis of the Hilbert space of operators acting on the OQS. The following master equation is obtained for the dynamics of the reduced density matrix of the system

$$\frac{d}{dt}\rho_S(t) = -i[H(t), \rho_s(t)] + \sum_{k=1}^{N^2-1} \gamma_k(t) \left(A_k(t) \rho_S(t) A_k^\dagger(t) - \frac{1}{2}\{A_k^\dagger(t) A_k(t), \rho_S(t)\} \right) , \tag{31}$$

where N is again the dimension of the Hilbert space $\mathcal{H}_S$, but now the operators $A_k(t) \in \mathcal{H}_E$ and the decay rates $\gamma_k(t)$ are time dependent. This is a non-Markovian generalization of the Lindblad Eq. (29). Note that this equation can recover the canonical Markovian equation if $\gamma_k(t) \geq 0$, but that is not true in general. What is clear is that complete positivity cannot be achieved if the decay rates are negative, and during the time intervals where $\gamma_k(t) < 0$ non-Markovian behavior will be present.

There are many proposed measures to quantify the degree of non-Markovianity, some are based on the divisibility and complete positivity properties of the dynamical map and others on the distinguishability of states. Each measure has their respective pros and cons, and some are more suitable to describe some particular situations, but here we present the one that is the most commonly used.

4.1 A non-Markovianity measure

The measure proposed by [12] quantifies the distinguishability of states, via the rate of change of the trace distance. The trace distance between two states is defined as

$$D(\rho_1, \rho_2) = \frac{1}{2}\mathrm{Tr}|\rho_1 - \rho_2| \ , \tag{32}$$

where $|A| = \sqrt{AA^\dagger}$. The properties that make this measure appropriate for quantifying non-Markovianity are the following.

- Trace distance is preserved for unitary operations: $D(U\rho_1 U^\dagger, U\rho_2 U^\dagger) = D(\rho_1, \rho_2)$, where U is a unitary transformation.
- All CPT maps reduce the trace distance between two states that are subjected to the same map: $D(\phi\rho_1, \phi\rho_2) \leq D(\rho_1, \rho_2)$, where ϕ is a completely positive trace preserving map. This mean that any CPT map cannot increase the trace distance between two states.

The physical interpretation of this distance is that it constitutes a measure of state distinguishability. The rate of change of state distinguishability can be interpreted as a flow of information between the open system and the environment. A CPT map will always reduce the trace distance, and therefore a flow of information from the system onto the environment is produced. The first property indicates that for closed systems (those that undergo unitary evolution) the information is preserved.

For a Markovian process, information continuously flows outside the system. To have non-Markovian effects, there should be some time intervals where information flows back to the system. The rate of change of trace distance is defined as

$$\sigma(t, \rho_{1,2}(0)) = \frac{d}{dt} D(\rho_1(t), \rho_2(t)) \ , \tag{33}$$

where $\rho_{1,2}(t) = \phi(t)\rho_{1,2}(0)$. For a non-Markovian map $\phi(t)$ where at some intervals the information flows back to the open system we must have $\sigma > 0$ for these intervals. The measure for non-Markovianity as introduced by [12] should characterize the total amount of information flowing from the environment back to the system. It is suggested to define the measure $N(\phi)$ for the non-Markovianity of a quantum process described by $\phi(t, 0)$ as

$$N(\phi) = \max_{\rho_{1,2}(0)} \int_{\sigma>0} dt \sigma(t, \rho_{1,2}(0)) \ . \tag{34}$$

This definition of non-Markovianity has the drawback that it requires to find the two initial states $\rho_{1,2}(0)$ that maximize $N(\phi)$.

5 Derivation of a weak coupling ME

There are many procedures to obtain a ME for the dynamics of the reduced system, that is, the OQS density matrix. We are going to take the approach of a weak coupling between the system and the environment. Suppose that $H_I(t)$ is proportional to a coupling constant which we will denote in a generic way as g. This approach is equivalent to the one in which assumptions in the decay time scales of the system and environment are considered (*first* Markov approximation), as well as the consideration that the system and environment are not only initially uncorrelated, but also throughout the whole evolution (Born approximation). In our case, we consider that the OQS and the environment are only initially uncorrelated, that is, $\rho(0) = \rho_S(0) \otimes \rho_E(0)$.

We begin by considering Eq. (21) in the interaction picture and plugging it in the r.h.s. of Eq. (20) for $t_0 = 0$,

$$\frac{d}{dt}\hat{\rho}_S(t) = -i\mathrm{Tr}_E\left[V_t^0 H_I(t), \hat{\rho}(0)\right] - \int_0^t d\tau\ \mathrm{Tr}_E\left[V_t^0 H_I(t), \left[V_\tau^0 H_I(\tau), \hat{\rho}(\tau)\right]\right]\ , \tag{35}$$

which is an exact second order equation, $O(g^2)$. Now, if we take a further step and integrate both sides of this equation, we get

$$\hat{\rho}_S(t) = \hat{\rho}_S(0) - i\int_0^t d\tau\ \mathrm{Tr}_E\left[V_t^0 H_I(\tau), \hat{\rho}(0)\right] - \int_0^t ds \int_0^t d\tau\ \mathrm{Tr}_E\left[V_s^0 H_I(s), \left[V_\tau^0 H_I(\tau), \hat{\rho}(\tau)\right]\right]\ . \tag{36}$$

We now insert this into Eq. (20) and **keep only terms up to second order** to obtain

$$\frac{d}{dt}\hat{\rho}_S(t) = -i\mathrm{Tr}_E\left[V_t^0 H_I(t), \hat{\rho}(0)\right] - \int_0^t d\tau\ \mathrm{Tr}_E\left[V_t^0 H_I(t), \left[V_\tau^0 H_I(\tau), \hat{\rho}(0)\right]\right] + O(g^3)\ , \tag{37}$$

which is now an **approximate equation** for $\hat{\rho}_S(t)$. Note that this approximate equation is very similar to Eq. (35), with the difference that the total density matrix, in the last term, is now in the initial state. This is similar to a Markovian approximation in the sense that the past evolution of the density matrix is being ignored, and only its initial state is taken into account.

In most situations, as in this work, an environment composed by harmonic oscillators will be considered. If we consider a linear theory, which is usually the case, the interaction Hamiltonian will be linear in the creation and annihilation operators of the environment, that is, to have $B \propto a_\lambda$ in Eq. (3). The first term in the r.h.s. of Eq. (37) will be null, as it represents the expectation value of single annihilation or creation operators of the bosonic reservoir, which are always zero independently of the state of the bosonic bath (See explicit calculation in Appendix A.1). We therefore obtain

$$\frac{d}{dt}\hat{\rho}_S(t) = -\int_0^t d\tau\ \mathrm{Tr}_E\left[V_t^0 H_I(t), \left[V_\tau^0 H_I(\tau), \hat{\rho}(0)\right]\right]\ , \tag{38}$$

that can be formally integrated as before to lead to

$$\hat{\rho}_S(t) = \hat{\rho}_S(0) - \int_0^t ds \int_0^t d\tau\ \mathrm{Tr}_E\left[V_s^0 H_I(s), \left[V_\tau^0 H_I(\tau), \hat{\rho}(0)\right]\right]\ , \tag{39}$$

which implies that $\hat{\rho}_S(t) = \hat{\rho}_S(0) + O(g^2)$. We first see that

$$V_t^0 H_I = e^{iH_0 t}(LB^\dagger + L^\dagger B)e^{-iH_0 t}\ , \tag{40}$$

where $H_0 = H_S + H_E$ and $[H_S, H_E] = 0$, can be expressed as

$$V_t^0 H_I = e^{iH_S t} L e^{-iH_S t}\ e^{iH_E t} B^\dagger e^{-iH_E t} + e^{iH_S t} L^\dagger e^{-iH_S t}\ e^{iH_E t} B e^{-iH_E t}\ . \tag{41}$$

Making use of the definitions $V_t L = e^{iH_S t} L e^{-iH_S t}$ and $B(t) = e^{iH_E t} B e^{-iH_E t}$ the latter equation can be rewritten as

$$V_t^0 H_I = V_t L\ B^\dagger(t) + V_t L^\dagger\ B(t)\ . \tag{42}$$

Making use of these definitions and operating the r.h.s. term of Eq. (38) (See Appendix A.2 for a detailed calculation) leads to

$$\begin{aligned}
\frac{d}{dt}\hat{\rho}_S(t) = &\int_0^t d\tau \mathrm{Tr}_E\{B(t)^\dagger B(\tau)\hat{\rho}_E(0)\}\left[V_\tau L^\dagger \hat{\rho}_S(0), V_t L\right] \\
&+ \int_0^t d\tau \mathrm{Tr}_E\{B^\dagger(\tau) B(t)\hat{\rho}_E(0)\}\left[V_t L, \hat{\rho}_S(0) V_\tau L^\dagger\right] \\
&+ \int_0^t d\tau \mathrm{Tr}_E\{B(t) B^\dagger(\tau)\hat{\rho}_E(0)\}\left[V_\tau L \hat{\rho}_S(0), V_t L^\dagger\right] \\
&+ \int_0^t d\tau \mathrm{Tr}_E\{B(\tau) B^\dagger(t)\hat{\rho}_E(0)\}\left[V_t L^\dagger, \hat{\rho}_S(0) V_\tau L\right]\ .
\end{aligned} \tag{43}$$

We can now define the correlation functions, which encode the action of the environment, in the following way

$$\begin{aligned}
\alpha^+(t,\tau) &= \mathrm{Tr}_E\{B(t)^\dagger B(\tau)\hat{\rho}_E(0)\} \\
\alpha^-(t,\tau) &= \mathrm{Tr}_E\{B(t) B^\dagger(\tau)\hat{\rho}_E(0)\}\ ,
\end{aligned} \tag{44}$$

to rewrite (43) as

$$\begin{aligned}
\frac{d}{dt}\hat{\rho}_S(t) = &\int_0^t d\tau \alpha^+(t,\tau)\left[V_\tau L^\dagger \hat{\rho}_S(0), V_t L\right] \\
&+ \int_0^t d\tau \alpha^{+*}(t,\tau)\left[V_t L, \hat{\rho}_S(0) V_\tau L^\dagger\right] \\
&+ \int_0^t d\tau \alpha^-(t,\tau)\left[V_\tau L \hat{\rho}_S(0), V_t L^\dagger\right] \\
&+ \int_0^t d\tau \alpha^{-*}(t,\tau)\left[V_t L^\dagger, \hat{\rho}_S(0) V_\tau L\right]\ .
\end{aligned} \tag{45}$$

Recall that $\hat{\rho}_S(t) = \hat{\rho}_S(0) + O(g^2)$, which allows to substitute $\hat{\rho}_S(0)$ by $\hat{\rho}_S(t)$ and still have an equation valid up to second order in the coupling strength. Finally, if we apply the previous change and switch to the Schrödinger picture (See Appendix A.3 for the detailed procedure), we get the final equation for the dynamics of the OQS in the weak coupling limit

$$
\begin{aligned}
\frac{d}{dt}\rho_S(t) = & -i\left[H_S, \rho_S(t)\right] \\
& + \int_0^t d\tau \alpha^+(t,\tau)\left[V_{\tau-t}L^\dagger \rho_S(t), L\right] \\
& + \int_0^t d\tau \alpha^{+*}(t,\tau)\left[L, \rho_S(t) V_{\tau-t}L^\dagger\right] \\
& + \int_0^t d\tau \alpha^-(t,\tau)\left[V_{\tau-t}L\rho_S(t), L^\dagger\right] \\
& + \int_0^t d\tau \alpha^{-*}(t,\tau)\left[L^\dagger, \rho_S(t) V_{\tau-t}L\right] \ . \qquad (46)
\end{aligned}
$$

This equation has a similar structure to that of Eqs. (29) and (30), with a free evolution term, i.e., the first r.h.s. term in (46), and a dissipator, the remaining 4 terms. There is a difference though, the dynamical map described by this ME is by no means a Markovian map. The Markov limit could be recovered if the $V_t L$ terms evolve very slowly so that the integration limits in (46) can be extended to infinity (*second* Markov approximation). But complete positivity and the semigroup property are not in general recovered and the secular approximation has to be considered. The secular approximation consists on discarding fast oscillating terms at the level of the master equation and not in the interaction Hamiltonian, as was the case of the RWA. In some situations the secular and the RWA may be the same. Making use of theses approximations the ME can be recast into the canonical Lindblad form. We stress the fact that Eq. (46) is a non-Markovian master equation for the dynamics of the reduced density matrix of the OQS.

In the following sections we are going to describe different models where the above ME can be used to solve the dynamics of the OQS. All the models are going to be of the nature of the spin-boson model introduced in section 2.1. First of all, we present the Weisskopf-Wigner theory of spontaneous decay, a well-known spin-boson model which is exactly solvable under the RWA, and will be used to check whether the ME solution derived before is in good agreement with the exact solution. Then we will introduce two more models in which the environment is in a thermal state and have a more complex structure.

6 Weisskopf-Wigner theory of spontaneous decay

The Weisskopf-Wigner theory of spontaneous emission between two atomic levels was introduced to describe the phenomenological decay of an atom in an exited state to the ground state in a characteristic lifetime. This theory considers a continuum of field modes to properly describe atomic decay: if only one mode is considered, there would be an oscillation between the two levels of the system. This model is described by the total Hamiltonian

$$H = \frac{1}{2}\omega_0\sigma_z + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda + \sum_\lambda \left(g_\lambda^* \sigma_- a_\lambda^\dagger + g_\lambda \sigma_+ a_\lambda \right) \ , \tag{47}$$

as described in section 2.1 under the RWA.

6.1 Exact solution

The exact solution of this model can be found in multiple textbooks, we followed the one developed in [1]. The initial vacuum state of the environment allows to introduce the following states

$$\begin{aligned} |\psi_0\rangle &= |-\rangle_S \otimes |0\rangle_E \ , & (48)\\ |\psi_1\rangle &= |+\rangle_S \otimes |0\rangle_E \ , & (49)\\ |\psi_\lambda\rangle &= |-\rangle_S \otimes |\lambda\rangle_E \ , & (50) \end{aligned}$$

where $|\pm\rangle_S$ indicate the upper/lower level of the OQS, the state $|0\rangle$ denotes the vacuum state of the reservoir and $|\lambda\rangle_E = a_\lambda^\dagger |0\rangle_E$ is the state with one photon in the mode λ. The total state of the system has the form

$$|\psi(t)\rangle = c_0(t)\,|\psi_0\rangle + c_1(t)\,|\psi_1\rangle + \sum_\lambda c_\lambda(t)\,|\psi_\lambda\rangle \ , \tag{51}$$

where $c_X(t)$ are the amplitudes of each state. The Schrödinger equation for this state in the interaction picture is

$$\frac{d}{dt}|\psi(t)\rangle = -i\hat{H}_I(t)\,|\psi(t)\rangle \ , \tag{52}$$

where $\hat{H}_I(t) = \sum_\lambda \left(g_\lambda \sigma_+ a_\lambda e^{i(\omega_0-\omega_\lambda)t} + g_\lambda^* \sigma_- a_\lambda^\dagger e^{-i(\omega_0-\omega_\lambda)t} \right)$ and acts on $|\psi(t)\rangle$ as

$$\hat{H}_I(t)\,|\psi(t)\rangle \begin{cases} \hat{H}_I(t)\,|\psi_0\rangle = 0 \ , \\ \hat{H}_I(t)\,|\psi_1\rangle = \sum_\lambda g_\lambda^* e^{-i(\omega_0-\omega_\lambda)t}\,|\psi_\lambda\rangle \ , \\ \hat{H}_I(t)\,|\psi_\lambda\rangle = \sum_{\lambda'} g_{\lambda'} e^{i(\omega_0-\omega_{\lambda'})t}\sigma_+\,|-\rangle_S \otimes a_{\lambda'}\,|\lambda\rangle_E = g_\lambda e^{i(\omega_0-\omega_\lambda)t}\,|\psi_1\rangle \ , \end{cases} \tag{53}$$

where $a_{\lambda'}\,|\lambda\rangle = \delta_{\lambda',\lambda}\,|0\rangle_E$, $\sigma_+\,|-\rangle = |+\rangle$ and $\sigma_-\,|+\rangle = |-\rangle$. Equating the factors that multiply the same state in both sides of Eq. (52) we end up with the following system of ordinary differential equations

$$\begin{aligned} \dot{c}_0(t) &= 0 \ , & (54)\\ \dot{c}_1(t) &= -i\sum_\lambda g_\lambda e^{i(\omega_0-\omega_\lambda)t} c_\lambda(t) \ , & (55)\\ \dot{c}_\lambda(t) &= -i g_\lambda^* e^{-i(\omega_0-\omega_\lambda)t} c_1(t) \ . & (56) \end{aligned}$$

We assumed that the reservoir was initially in the vacuum state $c_k(0) = 0$. Solving the third equation and inserting it into the second we get a closed equation for $c_1(t)$,

$$\dot{c}_1(t) = -\int_0^t d\tau \sum_\lambda |g_\lambda|^2 e^{-i\omega_\lambda(t-\tau)} e^{i\omega_0(t-\tau)} c_1(t) \ , \tag{57}$$

where, if we make use of the definitions (12) and (13), we can write

$$\sum_\lambda |g_\lambda|^2 e^{-i\omega_\lambda(t-\tau)} = \frac{1}{\pi} \int d\omega J(\omega) e^{-i\omega(t-\tau)} = \alpha(t-\tau) \ , \tag{58}$$

and re-express Eq. (57),

$$\dot{c}_1(t) = -\int_0^t d\tau \alpha(t-\tau) e^{i\omega_0(t-\tau)} c_1(t) \ . \tag{59}$$

Note that, in this case, $\alpha(t-\tau) = \mathrm{Tr}_E\{B(t)B^\dagger(\tau)\rho_E(0)\}$, with $\rho_E(0) = (|0\rangle\langle 0|)_E$ the vacuum state of the reservoir. We are now prepared to obtain the reduced density matrix dynamics of the two level system (TLS) from the the total density matrix $\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|$,

$$\hat{\rho}_S(t) = \mathrm{Tr}_E\{|\psi(t)\rangle\langle\psi(t)|\} = \begin{pmatrix} \rho_{++}(t) & \rho_{+-}(t) \\ \rho_{-+}(t) & \rho_{--}(t) \end{pmatrix} = \begin{pmatrix} |c_1(t)|^2 & c_o^* c_1(t) \\ c_0 c_1^*(t) & 1 - |c_1(t)|^2 \end{pmatrix} \ , \tag{60}$$

where the matrix is expressed in the basis $\{|\pm\rangle\}$ of the TLS, so that, for example, $\rho_{++}(t) = \langle +|\rho_S|+\rangle$, and the normalization condition $|c_o|^2 + |c_1(t)|^2 + \sum_\lambda |c_\lambda(t)|^2 = 1$ has been used in the last element of the matrix. By direct differentiation of Eq. (60) with respect to time we obtain an equation with the same structure as Eq. (31)

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{i}{2} S(t) \left[\sigma_+\sigma_-, \hat{\rho}_S(t)\right] + \gamma(t) \left(\sigma_- \hat{\rho}_S(t) \sigma_+ - \frac{1}{2}\{\sigma_+\sigma_- \hat{\rho}_S(t)\} \right) \ , \tag{61}$$

where we introduced the definitions

$$S(t) = -2\mathrm{Im}\left(\frac{\dot{c}_1(t)}{c_1(t)}\right) \ , \quad \text{and} \quad \gamma(t) = -2\mathrm{Re}\left(\frac{\dot{c}_1(t)}{c_1(t)}\right) \ , \tag{62}$$

representing a time-dependent "Lamb shift" and decay rate, respectively. If we switch to the Schrödinger picture, neglecting the Lamb shift, and express Eq. (61) in terms of each component of the density matrix, we get the following system of differential equations

$$\dot{\rho}_{++}(t) = -\rho_{++}(t)\gamma(t) \ , \tag{63}$$

$$\dot{\rho}_{--}(t) = \rho_{++}(t)\gamma(t) \ , \tag{64}$$

$$\dot{\rho}_{+-}(t) = -i\omega_0\rho_{+-}(t) - \frac{1}{2}\rho_{+-}(t)\gamma(t) \ . \tag{65}$$

It is useful to define the new quantity $G(t) = \frac{c_1(t)}{c_1(0)}$, which is described by the equation

$$\dot{G}(t) = -\int_0^t d\tau \alpha(t-\tau) e^{i\omega_0(t-\tau)} G(t) \ , \tag{66}$$

with initial condition $G(0) = 1$, which is independent of the initial state of the TLS, in opposition to Eq. (57).

We consider the Jaynes-Cummings model (JCM) which describes a two level atom coupled to a single cavity mode, which in turn is coupled to a series of harmonic oscillators that are initially in the vacuum state. If we restrict the model to the case of single exitations in the atom-cavity system, the cavity mode can be eliminated and we have the effective Hamiltonian of Eq. (47). We consider the case in which the atom transition frequency and the cavity mode are resonant, although the case in which they were detuned would be similar. The spectral density function that describes the effect of the electromagnetic reservoir is the Breit-Wigner distribution

$$J(\omega) = \frac{1}{2} \frac{\gamma_0 \lambda^2}{(\omega - \omega_0)^2 + \lambda^2} , \tag{67}$$

where ω_0 is the transition frequency of the TLS. The parameter λ defines the spectral width of the coupling and γ_0 defines to the decay rate of the TLS. This spectral density gives rise to the exponential decay law of the environment correlations, which is observed experimentally, when the integration over the frequencies is extended from $-\infty$ to $+\infty$ [13] in the calculation of the correlation function (58). This fact can be viewed as if the negative frequencies had a physical meaning because of the squared difference in Eq. (67). If we were treating the case in which the cavity frequency ω_{cav} and the transition frequency of the TLS were not in resonance, the above distribution would be modified by the addition of the detuning parameter $\Delta = \omega_0 - \omega_{cav}$,

$$J(\omega) = \frac{1}{2} \frac{\gamma_0 \lambda^2}{(\omega - \omega_0 + \Delta)^2 + \lambda^2} . \tag{68}$$

The correlation function (58) for the spectral density function (67) is given by

$$\alpha(t - \tau) = \frac{1}{2} \lambda \gamma_0 e^{-\lambda |t-\tau|} e^{-i\omega_0 (t-\tau)} . \tag{69}$$

For this correlation function, Eq. (66) becomes

$$\dot{G}(t) = - \int_0^t d\tau f(t-\tau) G(t) , \tag{70}$$

where we defined $f(t-\tau) = \frac{1}{2}\lambda\gamma_0 e^{-\lambda|t-\tau|}$, and can be analytically solved by means of the Laplace transform. The Laplace transform of Eq. (70) is

$$s\hat{G}(s) - G(0) = -\hat{f}(s)\hat{G}(s) , \tag{71}$$

where $\hat{G}(s)$ and $\hat{f}(s)$ are the Laplace transformations of $G(t)$ and $f(t)$, respectively. Making use of the initial condition $G(0) = 1$ and solving for $\hat{G}(s)$ we get

$$\hat{G}(s) = \frac{1}{s - \hat{f}(s)} , \tag{72}$$

where

$$\hat{f}(s) = \frac{1}{2} \gamma_0 \frac{\lambda}{\lambda + s} , \tag{73}$$

is the Laplace transform of $f(t)$ defined before. Applying the inverse Laplace transform to Eq. (72) yields the following exact result

$$G(t) = e^{-\lambda t/2} \left[\cosh\left(\frac{dt}{2}\right) + \frac{\lambda}{d} \sinh\left(\frac{dt}{2}\right) \right] , \tag{74}$$

where the variable $d = \sqrt{\lambda^2 - 2\lambda\gamma_0}$ was introduced. For this function, the time-dependent decay rate (62) becomes

$$\gamma(t) = \frac{2\gamma_0\lambda\sinh(dt/2)}{d\cosh(dt/2) + \lambda\sinh(dt/2)} \; . \tag{75}$$

Note that the Lamb-shift would be null for this solution. The parameter d introduces a change of behavior in Eq. (75): if d is real, $\gamma(t)$ is a monotonous function, but if d is an imaginary number, $\gamma(t)$ oscillates. This behavior is determined by the coupling strength. For small couplings $\gamma_0 < \lambda/2$ we have a Markovian behavior of the system and a positive decay rate $\gamma(t) \geq 0$. For the strong coupling case $\gamma_0 > \lambda/2$ we have an oscillatory decay rate, and at some times it may become negative, yielding non-Markovian dynamics. In the case of the JCM there is a correspondence between the sign of the decay rate and non-Markovian behavior because the Lindblad operators in (61) are time independent, but in general that is not the case.

6.2 Weak ME solution

To obtain a differential equation for the dynamics of the reduced density matrix of the OQS we need to calculate the correlation functions and the commutators appearing in Eq. (46). We proceed to calculated the correlation functions in Eq. (44)

$$\alpha^{+}(t,\tau) = \mathrm{Tr}_E\{B^\dagger(t)B(\tau)\rho_E(0)\} = \sum_{\lambda,\lambda'} g^*_\lambda g_{\lambda'} e^{i\omega_\lambda t} e^{-i\omega_{\lambda'}\tau}\mathrm{Tr}_E\{\langle 0|a^\dagger_\lambda a_{\lambda'}|0\rangle\} = 0 \; , \tag{76}$$

where the cyclic property of the trace has been used, and also the fact that $a_\lambda\left|0\right\rangle = 0$. The other correlation function is

$$\begin{aligned} \alpha^{-}(t,\tau) = \mathrm{Tr}_E\{B(t)B^\dagger(\tau)\rho_E(0)\} &= \sum_{\lambda,\lambda'} g^*_\lambda g_{\lambda'} e^{i\omega_\lambda \tau} e^{-i\omega_{\lambda'} t}\left\langle 0|a_{\lambda'}a^\dagger_\lambda|0\right\rangle = \\ = \sum_{\lambda,\lambda'} g^*_\lambda g_{\lambda'} e^{i\omega_\lambda \tau} e^{-i\omega_{\lambda'} t}\Big(\delta_{\lambda,\lambda'} + \langle 0|a^\dagger_\lambda a_{\lambda'}|0\rangle\Big) &= \sum_\lambda |g_\lambda|^2 e^{-i\omega_\lambda(t-\tau)} \; , \end{aligned} \tag{77}$$

where the commutation relation $[a_\lambda, a^\dagger_{\lambda'}] = \delta_{\lambda,\lambda'}$ has been used. The same procedure as in Eq. (58) is carried out and considering the spectral function (67) yields the same correlation function as before (69). Given that the correlation function and the commutators in Eq. (46) for this model depend on the difference $t - \tau$ it is suitable to apply the change of variable $m = t - \tau$, so that $dm = -d\tau$ and the limits of integration become $\tau = 0 \implies m = t$ and $\tau = t \implies m = 0$. With this change of variable and the fact that $\alpha^{+}(t,\tau) = 0$, Eq. (46) becomes

$$\begin{aligned} \frac{d}{dt}\rho_S(t) = &-i\left[H_S, \rho_S(t)\right] \\ &+ \int_0^t dm\alpha^{-}(m)\left[V_{-m}L\rho_S(t), L^\dagger\right] \\ &+ \int_0^t dm\alpha^{-*}(m)\left[L^\dagger, \rho_S(t)V_{-m}L\right] \; . \end{aligned} \tag{78}$$

We left the calculation of the commutators to Appendix B.1 which will be useful later for others models. Splitting Eq. (78) into a system of ordinary differential equations for each

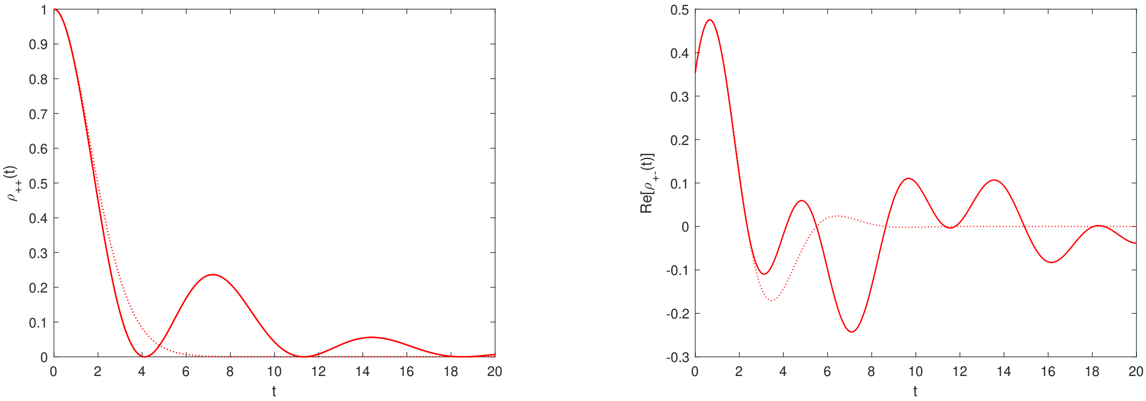


Figure 3: The left panel represents the upper population as a function of time. The solid line represent the exact solution, and the dashed one the solution of the ME. We clearly see that both solutions are in disagreement, as the ME solution only describes a decay, while the exact one has an initial decay followed by subsequent revivals. The same situation is true for the correlation function on the right panel. The parameters of these solutions are $\omega_0 = 1$, $\lambda = 0.2$ and $\gamma_0 = 10\lambda$. The units of λ, γ_0 and t are all relative to ω_0.

component of the density matrix leads to

$$\dot{\rho}_{++}(t) = -\rho_{++}(t) \int_0^t dm \left(\alpha^-(m) e^{i\omega_0 m} + \alpha^{-*}(m) e^{-i\omega_0 m} \right) \ , \tag{79}$$

$$\dot{\rho}_{--}(t) = \rho_{++}(t) \int_0^t dm \left(\alpha^-(m) e^{i\omega_0 m} + \alpha^{-*}(m) e^{-i\omega_0 m} \right) \ , \tag{80}$$

$$\dot{\rho}_{+-}(t) = -i\omega_0 \rho_{+-}(t) - \rho_{+-}(t) \int_0^t dm \alpha^-(m) e^{i\omega_0 m} \ . \tag{81}$$

Note that $\dot{\rho}_{++}(t) = -\dot{\rho}_{--}(t)$, which implies that the trace $\mathrm{Tr}_S \rho_S(t) = \rho_{++}(t) + \rho_{--}(t)$ will be preserved during the whole evolution, as the variation of one diagonal element is opposite to the other one. Substituting the expression for the correlation functions, which cancel out the exponential factors inside the integrals, and direct integration, lead to

$$\dot{\rho}_{++}(t) = -\rho_{++}(t)\gamma_0(1 - e^{-\lambda t}) \ , \tag{82}$$

$$\dot{\rho}_{--}(t) = \rho_{++}(t)\gamma_0(1 - e^{-\lambda t}) \ , \tag{83}$$

$$\dot{\rho}_{+-}(t) = -i\omega_0 \rho_{+-}(t) - \frac{1}{2}\rho_{+-}(t)\gamma_0(1 - e^{-\lambda t}) \ , \tag{84}$$

which is very similar to the system (63)-(65) for the exact solution with the difference of having a different (approximate) decay rate $\gamma'(t) = \gamma_0(1 - e^{-\lambda t})$.

6.3 Results

The implementation of Eqs. (63)-(65) of the exact solution for the decay (75) and Eqs. (82)-(84) of the ME solution in a numerical math program, for instance MATLAB, is straightforward. The parameter λ is related to the decay time, the higher the value of λ the faster the TLS system decays to the ground state, and the other way around. The paramater γ_0 presents also the same behaviour, but, as explained before, induces a change of behaviour depending on its relative value to λ. On the one hand, in the strong coupling regime

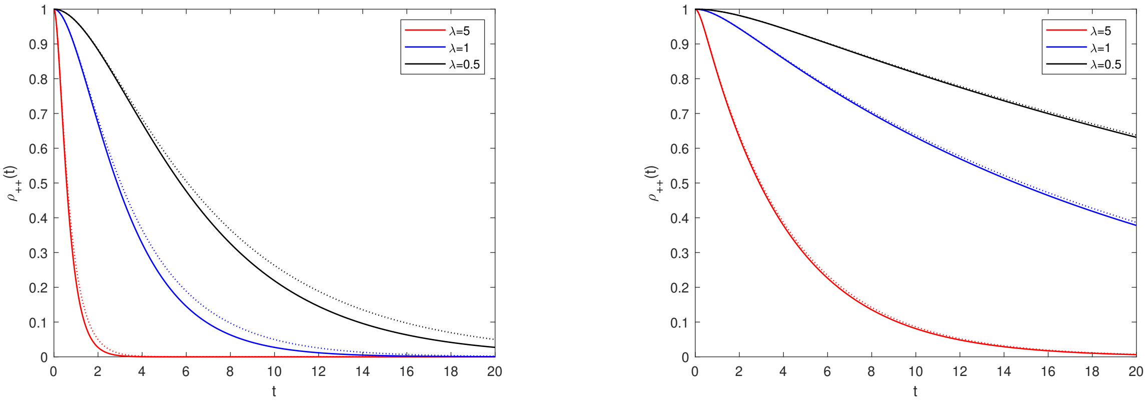


Figure 4: These panels represent the upper population for different values of λ shown in the legend. Again, solid lines represent the exact solution and dashed ones the ME solution. In the left panel we have plotted solution for a coupling $\gamma_0 = 1/3\lambda$ and in the right one for $\gamma_0 = 1/10\lambda$ for different λ. We clearly see that, the smaller the γ_0 is in comparison to λ the better is the agreement between solutions.

where $\gamma_0 > \lambda/2$ the exact and ME solutions have a very different behaviour, in Fig. 3 we compare the exact and the ME solutions, for both the upper popullation $\rho_{++}(t)$ and the correlation function $\rho_{+-}(t)$. We see that the population initially decays for both solutions, but the weak ME equation solution does not present the revivals that are present in the exact solution, hence the ME for this regime is not a good representation for the dynamics of the OQS. On the other hand, in the weak coupling limit $\gamma_0 < \lambda/2$, the weak ME solution closely matches the exact solution, and the match is even better when the ratio γ_0/λ is smaller, as seen in Fig. 4.

7 Pure dephasing mechanism

The pure dephasing mechanism is a very simple model proposed to investigate the effect of decoherence present in many quantum-mechanical systems. The physical situation in this case is the same as before, but we assume that no dissipation is present, that is, there is no transfer of energy between the OQS and the environment. This model is described by the same free Hamiltonian as the previous model and the following interaction Hamiltonian

$$H_I = \sigma_z \otimes \sum_\lambda (g_\lambda a_\lambda + g_\lambda^* a_\lambda^\dagger) \ , \tag{85}$$

where $\sigma_z = \sigma_+\sigma_- + \sigma_-\sigma_+$ does not yield transitions in the TLS.

7.1 Exact solution

The pure dephasing mechanism has been extensively studied to investigate the effect of decoherence and the exact solution can be found, for instance, in [14]. Since $[\sigma_z, H] = 0$ the populations of the TLS are not affected by the environment, i.e.,

$$\rho_{++}(t) = \rho_{++}(0) \tag{86}$$

$$\rho_{--}(t) = \rho_{--}(0) \ , \tag{87}$$

which can be explicitly checked by solving the full system. The evolution of the correlation term is

$$\rho_{+-}(t) = e^{-i\omega_0 t} e^{-\Gamma(t)} \rho_{+-}(0) \ , \tag{88}$$

where the exponential factor is given by

$$\Gamma(t) = -\frac{1}{2} \sum_\lambda |\xi_\lambda|^2 \ , \tag{89}$$

and

$$\xi_\lambda = 2g_\lambda \frac{1 - e^{i\omega_\lambda t}}{\omega_\lambda} \ . \tag{90}$$

We can operate the $\Gamma(t)$ factor by applying the continuum limit, which in a systematic way consists on making

$$\sum_\lambda |g_\lambda|^2 \to \frac{1}{\pi} \int d\omega J(\omega) \quad \text{and} \quad \omega_\lambda \to \omega \ , \tag{91}$$

leading to

$$\Gamma(t) = -\frac{1}{\pi} \int d\omega 4J(\omega) \frac{1 - \cos(\omega t)}{\omega^2} \ . \tag{92}$$

Making use of the spectral density (67) and direct integration of (92) completes the exact solution of this problem. The anallytic solution is quite involved but a numerical solution can be achieved easily.

7.2 Weak ME solution

The correlation function in this model do not differ from the previous JCM, as the environment is described by the same spectral density function. What will differ in this case is the form of the coupling between the OQS and the reservoir, given by a different expression of the commutators in Eq. (46), where now $L = L^\dagger = \sigma_z$. The explicit expression of these commutators is left out to Appendix B.2. The system of ordinary differential equations becomes

$$\dot{\rho}_{++}(t) = 0 \ , \tag{93}$$

$$\dot{\rho}_{--}(t) = 0 \ , \tag{94}$$

$$\dot{\rho}_{+-}(t) = -i\omega_0\rho_{+-}(t) - 2\rho_{+-}(t)\int_0^t dm\left(\alpha^-(m) + \alpha^{-*}(m)\right) \ , \tag{95}$$

where

$$\int_0^t dm\left(\alpha^-(m) + \alpha^{-*}(m)\right) = \int_0^t dm\frac{e^{i\omega_0 m} + e^{-i\omega_0 m}}{2}\lambda\gamma_0 e^{-\lambda m} = \frac{\lambda\gamma_0}{\lambda^2 + \omega_0^2}\left(\lambda - \lambda\cos\omega_0 t e^{-\lambda t} + \omega_0\sin\omega_0 t e^{-\lambda t}\right) \tag{96}$$

7.3 Results

A numerical solution of both the ME and analytic result lead to exactly the same evolution for the density matrix of the OQS. This happens because the ME assumes the evolution of the system operators L to be governed by the free Hamiltonian alone. In this case the exact evolution of the operator $L = \sigma_z$ is trivial, σ_z does not evolve, as well as in the case of the ME ($V_t L = L$), thats why both solutions coincide. This model is a nice example to check that the ME derived in section 5 does indeed represent well the evolution of the OQS.

8 Model A: Spin-$\frac{1}{2}$ coupled to a bosonic bath

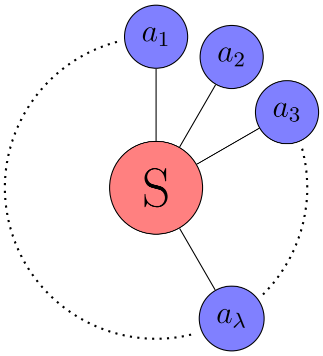


Figure 5: Schematic picture of Model A. The OQS is coupled, in a star configuration, to a set of harmonic oscillators a_λ.

Now we are going to present a model that describes a more realistic situation. We have the spin-$\frac{1}{2}$ system, that could be any quantum system under study whose degrees of freedom are two or can effectively be described as a TLS, coupled to a reservoir of harmonic oscillators that are at some finite temperature. The situation under study is depicted in Fig. 5. This model is very similar to the Weisskopf-Wigner theory described in Section 6 with the difference that the initial state of the reservoir is not the vacuum, but a thermal state at some finite temperature. This condition cannot be studied analytically and we have to recourse to the approximate method introduced in Section 5. The thermal state of the bath is

$$\rho_E^{therm}(0) = \frac{e^{-H_E\beta}}{\mathbb{Z}} \;, \tag{97}$$

where H_E is the free Hamiltonian of the bath, $\beta = (k_B T)^{-1}$ is the inverse temperature of the bath, with k_B the Boltzmann constant, and $\mathbb{Z} = \mathrm{Tr}_E e^{-H_E\beta}$ is called the partition function, which ensures the normalization of the density matrix. We need to compute the correlation functions that characterize this environment

$$\alpha^+(t,\tau) = \sum_{\lambda,\lambda'} g_\lambda^* e^{i\omega_\lambda t} g_{\lambda'} e^{-i\omega_{\lambda'}\tau} \mathrm{Tr}_E\{a_\lambda^\dagger a_{\lambda'} \rho_E^{therm}(0)\} \;, \tag{98}$$

and

$$\alpha^-(t,\tau) = \sum_{\lambda,\lambda'} g_\lambda e^{-i\omega_\lambda t} g_{\lambda'}^* e^{i\omega_{\lambda'}\tau} \mathrm{Tr}_E\{a_\lambda a_{\lambda'}^\dagger \rho_E^{therm}(0)\} \;. \tag{99}$$

To obtain the explicit form of the traces, we will make use of the cyclic property of the trace, the commutation relation between bosonic operators, and the commutation relation of the annihilation/creation operators with the thermal state,

$$[H_E, a_\lambda] = -\omega_\lambda a_\lambda \implies H_E a_\lambda = a_\lambda H_E - a_\lambda \omega_\lambda \;, \tag{100}$$

which can be generalized by induction to obtain

$$H_E^n a_\lambda = a_\lambda (H_E - \omega_\lambda)^n \;. \tag{101}$$

The thermal state can be written as

$$\rho_E^{therm}(0) = \frac{1}{\mathbb{Z}} \sum_n (-1)^n \frac{H_E^n \beta^n}{n!} \;, \tag{102}$$

so that, when making use of Eq. (101),

$$\rho_E^{therm}(0) a_\lambda = a_\lambda \rho_E^{therm}(0) e^{\omega_\lambda \beta} \ . \tag{103}$$

We are now set to calculate the trace

$$\mathrm{Tr}_E\{a_\lambda^\dagger a_{\lambda'} \rho_E^{therm}(0)\} = \mathrm{Tr}_E\{a_\lambda^\dagger \rho_E^{therm}(0) a_{\lambda'}\} e^{-\omega_{\lambda'}\beta} = \mathrm{Tr}_E\{a_{\lambda'} a_\lambda^\dagger \rho_E^{therm}(0)\} e^{-\omega_{\lambda'}\beta} \ , \tag{104}$$

where Eq. (103) has been used in the first identity and the cyclic property of the trace in the second one. Now making use of the commutation relation $[a_\lambda^\dagger, a_{\lambda'}] = \delta_{\lambda,\lambda'}$ we end up with

$$\mathrm{Tr}_E\{a_\lambda^\dagger a_{\lambda'} \rho_E^{therm}(0)\} = \Big(\mathrm{Tr}_E\{a_\lambda^\dagger a_{\lambda'} \rho_E^{therm}(0)\} + \delta_{\lambda,\lambda'} \mathrm{Tr}_E\{\rho_E^{therm}(0)\}\Big) e^{-\omega_{\lambda'}\beta} \ , \tag{105}$$

where the trace of the thermal state is identically unity. Solving for $\mathrm{Tr}_E\{a_\lambda^\dagger a_{\lambda'} \rho_E^{therm}(0)\}$ yields

$$\mathrm{Tr}_E\{a_\lambda^\dagger a_{\lambda'} \rho_E^{therm}(0)\} = \delta_{\lambda,\lambda'} \frac{1}{e^{\omega_{\lambda'}\beta} - 1} \equiv \delta_{\lambda,\lambda'} n(\omega_{\lambda'}) \ , \tag{106}$$

where the function $n(\omega_\lambda)$ is the average thermal number of quanta in the mode ω_λ at the inverse temperature β. A similar calculation is followed for the trace appearing in $\alpha^-(t,\tau)$. The correlation functions are simply

$$\alpha^+(t,\tau) = \sum_\lambda |g_\lambda|^2 n(\omega_\lambda) e^{i\omega_\lambda(t-\tau)} \ , \tag{107}$$

and

$$\alpha^-(t,\tau) = \sum_\lambda |g_\lambda|^2 \left(n(\omega_\lambda) + 1\right) e^{-i\omega_\lambda(t-\tau)} \ . \tag{108}$$

We can rewrite the above equations, in the continuum limit, as

$$\alpha^+(t,\tau) = \frac{1}{\pi} \int d\omega J(\omega) n(\omega) e^{i\omega(t-\tau)} \ , \tag{109}$$

$$\alpha^-(t,\tau) = \frac{1}{\pi} \int d\omega J(\omega) (n(\omega) + 1) e^{-i\omega(t-\tau)} \ , \tag{110}$$

where, for this model, we are going to use the spectral density function defined in Eq. (15) for the versatility it presents to describe different environments.

8.1 Weak Master Equation

The ME for this model, making use of the of the commutators calculated in Appendix B.1, becomes

$$\begin{aligned} \dot\rho_{++}(t) = & \int_0^t dm \big(\alpha^+(m)\rho_{--}(t) e^{-i\omega_0 m} + \alpha^{+*}(m)\rho_{--}(t) e^{i\omega_0 m} + \\ & + \alpha^-(m)(-\rho_{++}(t)) e^{i\omega_0 m} + \alpha^{-*}(m)(-\rho_{++}(t)) e^{-i\omega_0 m}\big) \ , \end{aligned} \tag{111}$$

$$\begin{aligned} \dot\rho_{--}(t) = - & \int_0^t dm \big(\alpha^+(m)\rho_{--}(t) e^{-i\omega_0 m} + \alpha^{+*}(m)\rho_{--}(t) e^{i\omega_0 m} + \\ & + \alpha^-(m)(-\rho_{++}(t)) e^{i\omega_0 m} + \alpha^{-*}(m)(-\rho_{++}(t)) e^{-i\omega_0 m}\big) \ , \end{aligned} \tag{112}$$

$$\dot\rho_{+-}(t) = -i\omega_0 \rho_{+-}(t) - \rho_{+-}(t) \int_0^t dm \left(\alpha^{+*}(m) + \alpha^-(m)\right) e^{i\omega_0 m} \ , \tag{113}$$

where the suitable change of variable $m = t - \tau$ was introduced, as $\alpha^{\pm}(t,\tau) = \alpha^{\pm}(t-\tau)$ and the commutators are functions of the difference $t-\tau$. Note that the trace is preserved along the evolution as $\dot{\rho}_{++}(t) = -\dot{\rho}_{--}(t)$. This fact, together with $\mathrm{Tr}\{\rho_S(t)\} = \rho_{++}(t) + \rho_{--}(t) = 1$, allows to substitute $\rho_{--}(t)$ by $1 - \rho_{++}(t)$, and reduce system (111)-(113) to a system of two differential equations

$$\dot{\rho}_{++}(t) = \int_0^t dm \left(\alpha^+(m)e^{-i\omega_0 m} + c.c.\right) - \rho_{++}(t)\int_0^t dm \left(\alpha^+(m)e^{-i\omega_0 m} + \alpha^-(m)e^{i\omega_0 m} + c.c.\right) , \tag{114}$$

$$\dot{\rho}_{+-}(t) = -\, i\omega_0\rho_{+-}(t) - \rho_{+-}(t)\int_0^t dm \left(\alpha^{+*}(m) + \alpha^-(m)\right) e^{i\omega_0 m} \ , \tag{115}$$

where *c.c.* is the complex conjugate of the terms in each parenthesis.

8.2 Asymptotic state

The study of the asymptotic state of the OQS can give some insight on the outcome of the interaction between a system and its environment, while the evolution up to this asymptotic state is also very important. In the long time limit the OQS may reach a steady state defined as

$$\rho^{ss} = \lim_{t\to\infty} \rho_S(t) \ , \tag{116}$$

and characterized by the condition $\dot{\rho}^{ss} = 0$. If this state is diagonal in the energy eigenbasis, the steady state is also stationary. Relaxation describes the convergence of the asymptotic state to an arbitrary state for the OQS, while thermalization is the convergence to the thermal state of the OQS. Thermalization is expected for a second order weak coupling perturbative ME under the RWA, but that is not the case in general [15], for instance when the RWA is not considered. We check that, under the assumptions we took, the OQS is thermalized by the bath. We consider the asymptotic limit ($t \to \infty$) of Eq. (114)

$$0 = \int_0^\infty dm \left(\alpha^+(m)e^{-i\omega_0 m} + c.c.\right) - \rho_{++}^{ss}\int_0^\infty dm \left(\alpha^+(m)e^{-i\omega_0 m} + \alpha^-(m)e^{i\omega_0 m} + c.c.\right) \ , \tag{117}$$

where

$$\int_0^\infty dm \left(\alpha^+(m)e^{-i\omega_0 m} + c.c.\right) = \int_0^\infty dm \int_0^\infty d\omega J(\omega)n(\omega)e^{-\omega/\omega_c}\left(e^{i(\omega-\omega_0)m} + e^{-i(\omega-\omega_0)m}\right) \ , \tag{118}$$

with

$$\begin{aligned}\int_0^\infty dm \left(e^{i(\omega-\omega_0)m} + e^{-i(\omega-\omega_0)m}\right) &= \int_0^\infty dm e^{i(\omega-\omega_0)m} - \int_0^{-\infty} dm e^{i(\omega-\omega_0)m} = \\ &= \int_{-\infty}^{\infty} e^{i(\omega-\omega_0)m} = \delta(\omega-\omega_0) \ ,\end{aligned} \tag{119}$$

leading to

$$\int_0^\infty dm \left(\alpha^+(m)e^{-i\omega_0 m} + c.c.\right) = J(\omega_0)n(\omega_0)e^{-\omega_0/\omega_c} \ . \tag{120}$$

And, in a similar fashion,

$$\int_0^\infty dm \left(\alpha^-(m)e^{-i\omega_0 m} + c.c.\right) = J(\omega_0)(n(\omega_0)+1)e^{-\omega_0/\omega_c} \ . \tag{121}$$

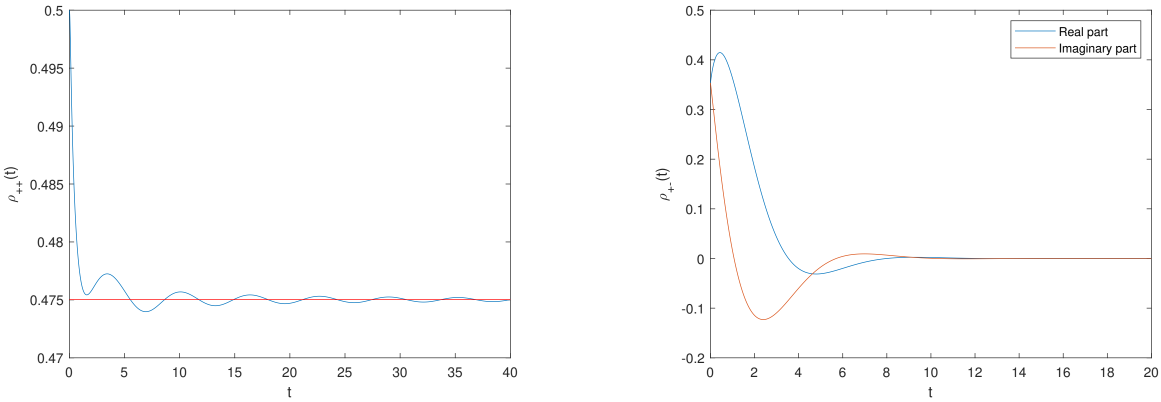


Figure 6: Dynamical evolution of model A for parameters $s = 1$, $\omega_c = 10$, $g = 0.01$ and $\beta = 0.1$. On the left panel we represent the upper popullation $\rho_{++}(t) = \langle +|\rho_S(t)|+\rangle$ in blue, and in red the value of ρ_{++}^{therm} of the thermal state. On the right panel we represented the correlation function $\rho_{+-}(t)$, both the real and imaginary part, in order to show that the OQS undergoes decoherence. From these plots we clearly see that the OQS thermalizes to the thermal state corresponding to the environment temperature. The initial conditions for these plots are $\rho_{++}(0) = \frac{1}{2}$ and $\rho_{+-}(0) = \frac{1}{2}\frac{(1+i)}{\sqrt{2}}$.

Now solving for ρ_{++}^{ss} in Eq. (117) leads to

$$\rho_{++}^{ss} = \frac{J(\omega_0)n(\omega_0)e^{-\omega_0/\omega_c}}{J(\omega_0)n(\omega_0)e^{-\omega_0/\omega_c} + J(\omega_0)(n(\omega_0)+1)e^{-\omega_0/\omega_c}} = \frac{n(\omega_0)}{2n(\omega_0)+1} \;, \tag{122}$$

where a direct calculation yields

$$\rho_{++}^{ss} = \frac{e^{-\beta\omega_0/2}}{e^{\beta\omega_0/2} + e^{-\beta\omega_0/2}} \;, \quad \text{and} \quad \rho_{--}^{ss} = 1 - \rho_{++}^{ss} = \frac{e^{\beta\omega_0/2}}{e^{\beta\omega_0/2} + e^{-\beta\omega_0/2}} \;. \tag{123}$$

Similarly, the asymptotic limit of Eq. (115) becomes

$$0 = \rho_{+-}^{ss}\left(-i\omega_0 - \int_0^\infty dm\,\left(\alpha^{+*}(m) + \alpha^{-}(m)\right)e^{i\omega_0 m}\right) \;, \tag{124}$$

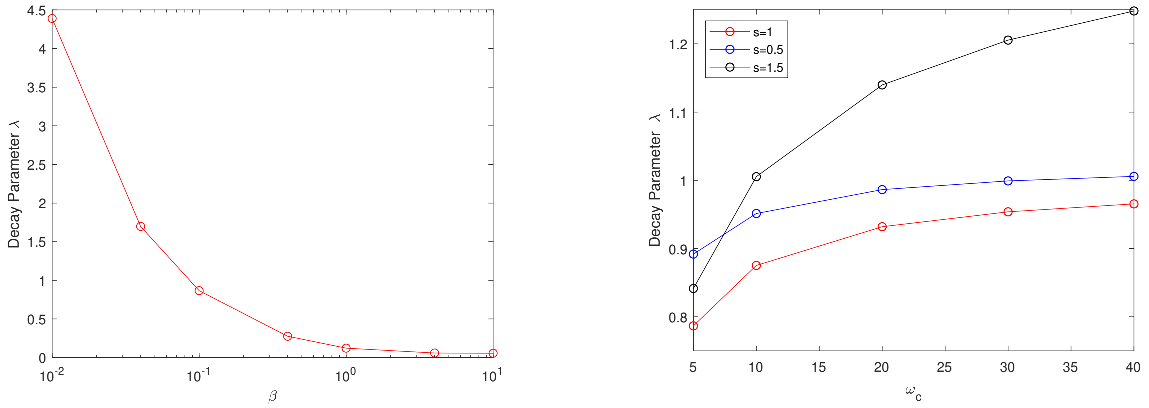
where one can check that the parenthesis in (124) does not vanish, so that the solution of this equation corresponds to $\rho_{+-}^{ss} = 0$. We can conclude that the asymptotic state of the Model A is the thermal state

$$\rho^{ss} = \frac{e^{-H_S\beta}}{\mathbb{Z}} = \rho_S^{therm} \;, \tag{125}$$

where β is the inverse temperature of the bath and $\mathbb{Z} = \mathrm{Tr}\{e^{-H_S\beta}\} = 2\cosh(\omega_0\beta/2)$.

8.3 Results

The numerical implementation of Eqs. (114) and (115) requires the calculation of the correlation functions $\alpha^{+}(m)$ and $\alpha^{-}(m)$. To calculate the correlation functions we have to do an integration along all the mode frequencies of the environment. Since the calculation of the correlation functions in the following model requires a discretization in frequencies, we can not just integrate to infinity. We choose a suitable ω_{max} and make sure that the



(a) $g = 0.01$, $s = 1$ and $\omega_c = 10$.

(b) $g = 0.01$ and $\beta = 0.1$.

Figure 7: Both panels represent the decay parameter λ obtained from the fit (126) for an initial condition $\rho_{++}(0) = 1$ as a function of some parameter of interest. The left panel shows a clear relationship between the inverse temperature of the reservoir and the thermalization time of the OQS. The right panel shows the λ parameter as a function of ω_c and s. The other paramaters of each plot are shown in the corresponding subcaptions.

result does not change if we increase it: this is satisfied if we set $\omega_{max} = 100\omega_0$. We do this in order to be consistent when comparing this model and model B. Apart from this detail, the integration to calculate the correlation functions is straightforward, as well as the numerical integration of the integrals appearing in (114) and (115) with the use of MATLAB implemented functions. An example of the dynamics of model A is plotted in Fig. 6, where it can easily be seen that the OQS thermalizes. To check how fast the OQS thermalizes, we performed the following fit for the dynamical curve of the upper population

$$\rho_{++}(t) = ae^{-\lambda t} + \rho_{++}^{therm} , \tag{126}$$

where the paramater λ indicates how fast the OQS decays. We run a number of simulations to investigate how the parameters in the spectral density affect the thermalization decay rate. In Fig. 7a we plotted the fit parameter λ as a function of the inverse temperature of the environment β. In all cases, the OQS achieves thermalization and we see that, the higher the temperature (small β) the faster the OQS thermalizes. This means that environments that are at higher temperatures quickly dissipate the OQS. This is the reason why quantum experiments, which require longer correlation times, are run at near zero temperatures, for instance in quantum computing. We also investigated how the width in modes of the reservoir ω_c and the parameter s affect the thermalization in Fig. 7b. We see that for the value $s = 1$, corresponding to a Ohmic bath, the thermalization is slower than for any other value. We also found that, the broader the spectrum is, the faster the OQS thermalizes.

9 Model B: Spin-$\frac{1}{2}$ coupled to a bosonic bath, which in turn is coupled to a second bosonic bath

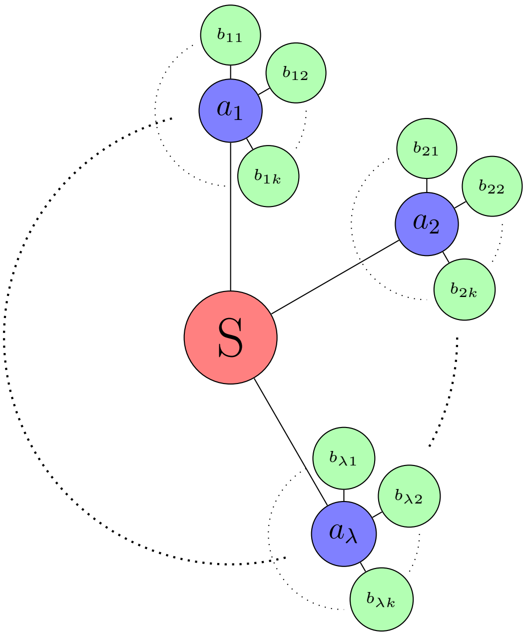


Figure 8: Schematic picture of Model B. The OQS is coupled in a star configuration to a set of harmonic oscillators a_λ, which are coupled to their own individual baths of harmonic oscillators $b_{\lambda k}$.

The standard scenario considered in the theory of OQS is that studied before, in which the open system is directly coupled to a single reservoir. However, it is not so well studied the situation where the OQS is coupled to a first reservoir (RI), that is in turn coupled to a second reservoir (RII). This second reservoir continuously thermalizes the first one, which in turn is taken out of equilibrium via its interaction with the OQS. We are going to consider the situation in which the harmonic oscillators in RI are coupled to the ones in RII in a star configuration, that is, each harmonic oscillator in RI has its own bath independent of the others, see Fig. 8 for a schematic picture. The Hamiltonian describing this situation is

$$H = \frac{1}{2}\omega_0\sigma_z + H_E + \sum_\lambda \left(g_\lambda^*\sigma_- a_\lambda^\dagger + g_\lambda\sigma_+ a_\lambda\right) \ , \tag{127}$$

where the Hamiltonian of the environment, H_E, is now more complex. It is composed by the free evolution of each bath, and an interaction term between them

$$H_E = \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda + \sum_{\lambda,k}\omega_{\lambda,k} b_{\lambda k}^\dagger b_{\lambda k} + \sum_{\lambda,k}\left(\tilde{g}_{\lambda k} a_\lambda b_{\lambda k}^\dagger + \tilde{g}_{\lambda k}^* a_\lambda^\dagger b_{\lambda k}\right) \ , \tag{128}$$

where $b_{\lambda k}$ are the harmonic oscillator operators with frequency $\omega_{\lambda,k}$ of RII coupled to the λ-th mode of RI and $\tilde{g}_{\lambda k}$ are the coupling strength constants between the harmonic oscillators in RI and RII. These operators obey the commutation relation $[b_{\lambda k}, b_{\lambda' k'}^\dagger] = \delta_{\lambda,\lambda'}\delta_{k,k'}$. Note that the decay of a bath mode in RI is accompanied by the creation of a boson in RII and viceversa.

We consider that RI and RII are initially uncorrelated and at different inverse temperatures β_1 and β_2, respectively. The initial state of the whole environment is $\rho_E(0) =$

$\rho_{RI}(0) \otimes \rho_{RII}(0)$. In this particular situation the correlation functions take the following form

$$\begin{aligned}
\alpha^{+}(t,\tau) &= \mathrm{Tr}_E\{B(t)^{\dagger}B(\tau)\rho_E(0)\} = \mathrm{Tr}_{I,II}\{B(t)^{\dagger}B(\tau)\left(\rho_{RI}(0)\otimes\rho_{RII}(0)\right)\} \\
\alpha^{-}(t,\tau) &= \mathrm{Tr}_E\{B(t)B^{\dagger}(\tau)\rho_E(0)\} = \mathrm{Tr}_{I,II}\{B(t)B^{\dagger}(\tau)\left(\rho_{RI}(0)\otimes\rho_{RII}(0)\right)\}\ ,
\end{aligned} \tag{129}$$

where $B(t) = \sum_\lambda g_\lambda a_\lambda(t) = \sum_\lambda g_\lambda e^{iH_E t} a_\lambda e^{-iH_E t}$ needs to be computed. The evolution of $a_\lambda(t)$ is given by

$$\frac{d}{dt}a_\lambda(t) = i\left[H_E, a_\lambda(t)\right] = -i\omega_\lambda a_\lambda(t) - i\sum_k \tilde{g}_{\lambda k} b_{\lambda k}(t)\ , \tag{130}$$

and the evolution of the opeators of RII is

$$\frac{d}{dt}b_{\lambda k}(t) = i\left[H_E, b_{\lambda k}(t)\right] = -i\omega_{\lambda,k} b_{\lambda k}(t) - i\tilde{g}_{\lambda k} a_\lambda(t)\ . \tag{131}$$

We can formally integrate the latter equation

$$b_{\lambda k}(t) = b_{\lambda k}(0)e^{-i\omega_{\lambda,k}t} - i\tilde{g}_{\lambda k}\int_0^t dt' a_\lambda(t')e^{-i\omega_{\lambda,k}(t-t')}\ , \tag{132}$$

and substitute this expression for $b_{\lambda k}(t)$ in (130) to yield

$$\frac{d}{dt}a_\lambda(t) = -i\omega_\lambda a_\lambda(t) - i\sum_k \tilde{g}_{\lambda k} b_{\lambda k}(0)e^{-i\omega_{\lambda,k}t} - \sum_k \tilde{g}_{\lambda k}^2 \int_0^t dt' e^{-i\omega_{\lambda,k}(t-t')}a_\lambda(t')\ . \tag{133}$$

We can see that the operator a_λ will oscillate with a frequency close to ω_λ. It is suitable to introduce the slow rotating variable

$$\tilde{a}_\lambda(t) = e^{i\omega_\lambda t}a_\lambda(t)\ , \tag{134}$$

which allows to correctly consider the Markovian limit. The evolution of the new variable is then

$$\frac{d}{dt}\tilde{a}_\lambda(t) = i\omega_\lambda\tilde{a}_\lambda(t) + \left(\frac{d}{dt}a_\lambda(t)\right)e^{i\omega_\lambda t}\ , \tag{135}$$

where, using the previous result (133), yields

$$\frac{d}{dt}\tilde{a}_\lambda(t) = -i\sum_k \tilde{g}_{\lambda k} b_{\lambda k}(0)e^{-i(\omega_{\lambda,k}-\omega_\lambda)t} - \sum_k \tilde{g}_{\lambda k}^2 \int_0^t dt' e^{-i(\omega_{\lambda,k}-\omega_\lambda)(t-t')}\tilde{a}_\lambda(t')\ . \tag{136}$$

The first term is the quantum noise of RII, and can be rewritten as $F_\lambda(t) = e^{i\omega_\lambda t}f_\lambda(t)$ with

$$f_\lambda(t) = -i\sum_k \tilde{g}_{\lambda k} b_{\lambda k}(0)e^{-i\omega_{\lambda,k}t}\ . \tag{137}$$

The integral in the last term of Eq. (136) can be simplified by considering that $\tilde{a}_\lambda(t')$ varies with a rate much slower than ω_λ, so that it can be taken out of the integral

$$\int_0^t dt' e^{-i(\omega_{\lambda,k}-\omega_\lambda)(t-t')}\tilde{a}_\lambda(t') \approx \tilde{a}_\lambda(t)\int_0^t dt' e^{-i(\omega_{\lambda,k}-\omega_\lambda)(t-t')}\ . \tag{138}$$

This is called the Weisskopf-Wigner approximation [2, 16], which can be ragarded as a Markovian approximation, as the dynamics of $\tilde{a}_\lambda(t)$ only depend on t and not on past instants of time. Since the time scale of the evolution of $\tilde{a}_\lambda(t)$ is much slower than the exponential inside the integral the integration limit can be extended to infinity and apply the Sokhotski–Plemelj theorem to get

$$\int_0^\infty d\tau e^{-i(\omega_{\lambda,k}-\omega_\lambda)\tau} = \pi\delta(\omega_{\lambda,k}-\omega_\lambda) - i\mathcal{P}\left(\frac{1}{\omega_{\lambda,k}-\omega_\lambda}\right) , \tag{139}$$

where we introduced the change of variable $\tau = t - t'$, and $\mathcal{P}$ is the Cauchy principal part. Making use of these approximations, the last term in Eq. (136) can be rewritten as

$$\sum_k \tilde{g}_{\lambda k}^2 \int_0^t dt' e^{-i(\omega_{\lambda,k}-\omega_\lambda)(t-t')}\tilde{a}_\lambda(t') \approx \gamma_\lambda \tilde{a}_\lambda(t) , \tag{140}$$

where we defined the damping constant

$$\gamma_\lambda = J_{II}(\omega_\lambda) - i\sum_k \tilde{g}_{\lambda k}^2 \mathcal{P}\left(\frac{1}{\omega_{\lambda,k}-\omega_\lambda}\right) , \tag{141}$$

and the spectral density of RII is defined as $J_{II}(\omega) = \pi\sum_k g_{\lambda k}^2 \delta(\omega_{\lambda,k}-\omega)$. The imaginary part in a decay rate plays the role of a frequency shift, it is in fact a contribution to the Lamb's shift, and we will neglect it. Making use of these definitions, we find that

$$\frac{d}{dt}\tilde{a}_\lambda(t) = -\gamma_\lambda \tilde{a}_\lambda(t) + F_\lambda(t) , \tag{142}$$

which can be analytically solved to give

$$\tilde{a}_\lambda(t) = \tilde{a}_\lambda(0)e^{-\gamma_\lambda t} + \int_0^t dt' e^{-\gamma_\lambda(t-t')}F_\lambda(t') , \tag{143}$$

and the evolution the original operator now reads

$$a_\lambda(t) = a_\lambda(0)e^{-(i\omega_\lambda+\gamma_\lambda)t} + \int_0^t dt' e^{-(i\omega_\lambda+\gamma_\lambda)(t-t')}f_\lambda(t') . \tag{144}$$

We are now set to compute the correlation functions (129) and first note that the first term in $a_\lambda(t)$ depends on $a_\lambda(0) = a_\lambda$, and the second one on operators on RII. When operating $a_\lambda(t)^\dagger a_\lambda(\tau)$ the terms lineal in operators of either RI or RII are null by reseasons explained before, but terms quadratic in these operators are not. The non-null terms of $\alpha^+(t,\tau)$ are

$$\begin{aligned}\alpha^+(t,\tau) &= \sum_{\lambda,\lambda'} g_\lambda^* g_{\lambda'} e^{(i\omega_\lambda-\gamma_\lambda)t} e^{(-i\omega_{\lambda'}-\gamma_{\lambda'})\tau} \mathrm{Tr}_{I,II}\{a_\lambda^\dagger a_{\lambda'}(\rho_{RI}(0)\otimes\rho_{RII}(0))\} \\ &+ \sum_{\lambda,\lambda'} g_\lambda^* g_{\lambda'} \int_0^t dt' \int_0^\tau dt'' e^{(i\omega_\lambda-\gamma_\lambda)(t-t')} e^{(-i\omega_{\lambda'}-\gamma_{\lambda'})(\tau-t'')} \mathrm{Tr}_{I,II}\{f_\lambda^\dagger(t') f_{\lambda'}(t'')(\rho_{RI}(0)\otimes\rho_{RII}(0))\},\end{aligned} \tag{145}$$

where

$$\mathrm{Tr}_{I,II}\{a_\lambda^\dagger a_{\lambda'}(\rho_{RI}(0)\otimes\rho_{RII}(0))\} = \mathrm{Tr}_I\{a_\lambda^\dagger a_{\lambda'}\rho_{RI}(0)\}\cancelto{1}{\mathrm{Tr}_{II}\{\rho_{RII}(0)\}} = \delta_{\lambda,\lambda'} n^I(\omega_\lambda) , \tag{146}$$

with $n^I(\omega_\lambda)$ the average thermal number of quanta in the mode ω_λ at the inverse temperature β_I of RI, as calculated for Model A. The other trace can be computed as

$$\sum_{k,k'} \tilde{g}^*_{\lambda k}\tilde{g}_{\lambda' k'} e^{i\omega_{\lambda,k}t'} e^{-i\omega_{\lambda',k'}t''} \mathrm{Tr}_{II}\{b^\dagger_{\lambda k}(0) b_{\lambda' k'}(0)\rho_{RII}(0)\} \ , \tag{147}$$

with

$$\mathrm{Tr}_{II}\{b^\dagger_{\lambda k}(0) b_{\lambda' k'}(0)\rho_{RII}(0)\} = n^{II}(\omega_{\lambda k})\delta_{\lambda,\lambda'}\delta_{k,k'} \ , \tag{148}$$

and, similarly, $n^{II}(\omega_{\lambda k})$ is the average thermal number of quanta of the k-th mode in the λ-th reservoir at the inverse temperature β_{II} of the RII. With the values of these traces, Eq. (145) reduces to

$$\begin{aligned}\alpha^+(t,\tau) = &\sum_\lambda |g_\lambda|^2 n^I(\omega_\lambda) e^{i\omega_\lambda(t-\tau)} e^{-\gamma_\lambda(t+\tau)} \\ &+ \sum_{\lambda,k} |g_\lambda|^2 |\tilde{g}_{\lambda k}|^2 n^{II}(\omega_{\lambda k}) \int_0^t dt' e^{-i(\omega_\lambda - \omega_{\lambda,k}+\gamma_\lambda)t'} \int_0^\tau dt'' e^{i(\omega_\lambda-\omega_{\lambda,k}+\gamma_\lambda)t''} e^{i\omega_\lambda(t-\tau)} e^{-\gamma_\lambda(t+\tau)} \ .\end{aligned} \tag{149}$$

Evaluating the integrals, using the definition $\Omega_{k,\lambda} = \omega_\lambda - \omega_{\lambda,k}$ and simplying leads to

$$\begin{aligned}\alpha^+(t,\tau) = &\sum_\lambda |g_\lambda|^2 n^I(\omega_\lambda) e^{i\omega_\lambda(t-\tau)} e^{-\gamma_\lambda(t+\tau)} \\ &+ \sum_{\lambda,k} |g_\lambda|^2 |\tilde{g}_{\lambda k}|^2 n^{II}(\omega_{\lambda k}) \left(\frac{e^{i\omega_{\lambda,k}t} - e^{(i\omega_\lambda - \gamma_\lambda)t}}{-i\Omega_{\lambda,k}+\gamma_\lambda}\right)\left(\frac{e^{-i\omega_{\lambda,k}\tau} - e^{(-i\omega_\lambda-\gamma_\lambda)\tau}}{i\Omega_{\lambda,k}+\gamma_\lambda}\right) \ .\end{aligned} \tag{150}$$

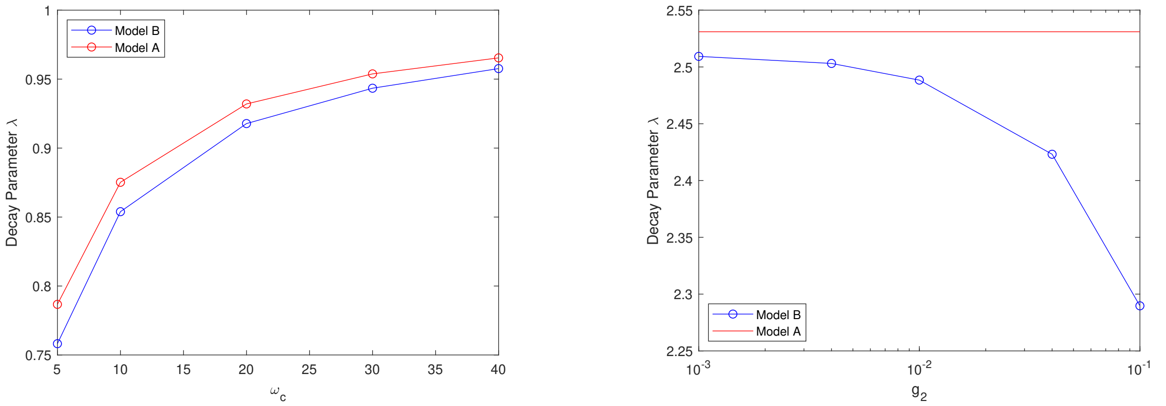
Similarly the remaining correlation function becomes

$$\begin{aligned}\alpha^-(t,\tau) = &\sum_\lambda |g_\lambda|^2 (n^I(\omega_\lambda)+1) e^{-i\omega_\lambda(t-\tau)} e^{-\gamma_\lambda(t+\tau)} \\ &+ \sum_{\lambda,k} |g_\lambda|^2 |\tilde{g}_{\lambda k}|^2 (n^{II}(\omega_{\lambda k})+1) \left(\frac{e^{-i\omega_{\lambda,k}t} - e^{(-i\omega_\lambda - \gamma_\lambda)t}}{i\Omega_{\lambda,k}+\gamma_\lambda}\right)\left(\frac{e^{i\omega_{\lambda,k}\tau} - e^{(i\omega_\lambda-\gamma_\lambda)\tau}}{-i\Omega_{\lambda,k}+\gamma_\lambda}\right) \ .\end{aligned} \tag{151}$$

The ME equations of this model looks like Eqs. (114) and (115) with the difference that the correlation functions, after the change of variable, are $\alpha^+(t, t-m)$ and $\alpha^-(t, t-m)$, which are now dependent of two variables t and m. After this change of variable and the continuum limit the correlation functions become

$$\begin{aligned}\alpha^+(t,t-m) = &\frac{1}{\pi}\int d\omega J_I(\omega) n^I(\omega) e^{i\omega m} e^{-J_{II}(\omega)(2t-m)} \\ &+ \frac{1}{\pi}\int d\omega \frac{1}{\pi}\int d\omega' J_I(\omega) J_{II}(\omega') n^{II}(\omega') \\ &\times \left(\frac{e^{i\omega' t} - e^{(i\omega - J_{II}(\omega))t}}{-i(\omega-\omega')+J_{II}(\omega)}\right)\left(\frac{e^{-i\omega'(t-m)} - e^{(-i\omega - J_{II}(\omega))(t-m)}}{i(\omega-\omega')+J_{II}(\omega)}\right) \ ,\end{aligned} \tag{152}$$

and similarly for $\alpha^-(t, t-m)$.



(a) $g = g_1 = g_2 = 0.01$, $s = s_1 = s_2 = 1$, $\omega_c = \omega_{c1} = \omega_{c2}$ and $\beta = \beta_1 = \beta_2 = 0.1$. Initial condition $\rho_{++}(0) = 1$.

(b) $g = g_1 = 0.01$, $s = s_1 = s_2 = 1$, $\omega_c = \omega_{c1} = \omega_{c2} = 10$ and $\beta = \beta_1 = \beta_2 = 0.1$. Initial condition $\rho_{++}(0) = 1/2$

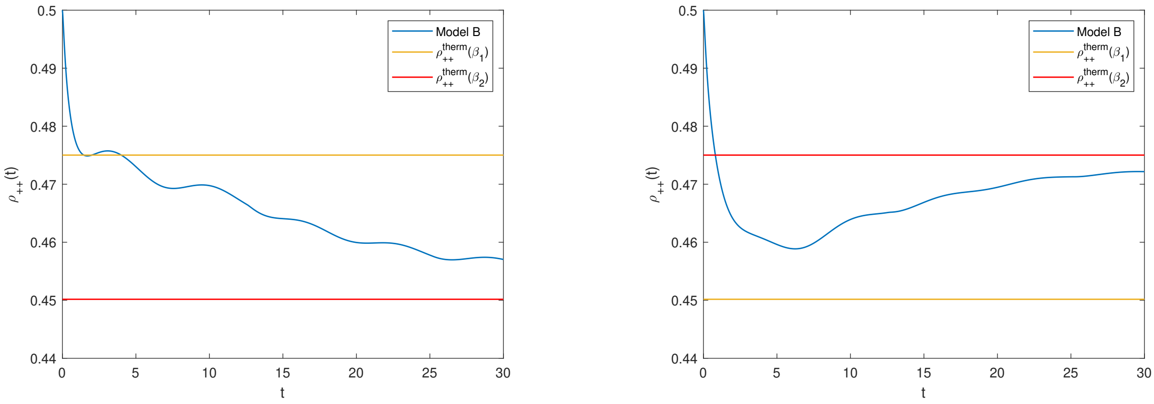
Figure 9: The left panel represents the decay rate towards thermalization as a function of ω_c for model A and B. A clear tendency is followed by both models, but model B does it at a lower rate. The right panel represents the thermalization rate as a function of the coupling between environments, g_2. When the coupling is stronger the OQS decays slower.

9.1 Numerical implementation

The ME for this model is exactly the same as for model A, the only difference resides in the correlation functions. To calculate the correlation functions, we had to develope a numerical code to first obtain a 2 dimensional grid with the values of the correlation functions $\alpha^{\pm}(t, m)$. To do this calculation, we divided the correlation function into two parts: one which is just a simple integral in ω (1st term in Eq. (152)) and a second that is a double integral (2nd term in Eq. (152)). The first term calculation is easy, as in the case of model A, the second one requires to first give discrete values to ω' from 0 to ω_{max} in intervals $\Delta\omega'$, and to obtain for each of this values the numerical integral with respect to ω in the same interval $\omega \in [0, \omega_{max}]$. Then we have to numerically integrate with respect to ω' each discrete value obtained. This process has to be repeated for each value of t and m. Note that since the integration of the correlation functions is from $m = 0$ to t we only have to calculate half the grid. The last operation that has to be performed is to multiply the correllation function by the different exponentials appearing in Eqs. (114) and (115) and numerically integrate along the dimension m of the grid. From this point on, any ODE solver of MATLAB is good at solving the ME. We parallelized all the *for* loops we could to reduce the simulation time, which for a typical simulation up to $t = 10$ takes half an hour.

9.2 Results

We explored what happens to the OQS when both reservoirs are at the same temperature, and also the case where the reservoirs are at a different temperature. In both cases we consider all the parameters, except the temperature, equal for both reservoirs, that is, both baths have the same s and the same bandwidth parametrized by ω_c. To be consistent with the approximations made to derive the correlation functions of model B, we take



(a) $\beta_1 < \beta_2$

(b) $\beta_1 > \beta_2$

Figure 10: The panel on the left represents the situation where the temperature of RI higher than the one of RII. The panel on the left represent the opposite situation. In both panels the blue line represents the evolution of the upper popullation of the OQS for the initial condition $\rho_{++}(0) = 1/2$. In red line is represented the upper population of the thermal state for β_2 and in orange for β_1. In both cases the OQS seems to thermalize to a thermal state with temperature β_2 of the RII.

a weak coupling constant between both reservoirs. We will denote by g_1 the coupling constant between the OQS and the first reservoir, and by g_2 the one between reservoirs.

When both thermal baths are at the same temperature we observe a similar behaviour as in model A, but since there is a structure between RI and RII the evolution of the OQS does not necessarily mimic the one in model A. The RI has to be in equilibrium for the OQS to be able to thermalize. Since the OQS takes out of equilibrium the RI and this one is in turn coupled to a RII, the equilibrium condition is harder to achieve. We carried out the same study as in model A for the decay rate towards the thermal state, as a function of the parameter ω_c. We took $\omega_{c1} = \omega_{c2} = \omega_c$. In Fig. 9a we plotted the comparison between the decay rate in model A and B. Both models follow the same tendency with ω_c, but in all cases the model A thermalizes faster than model B. This effect was checked for a value $g_2 = 0.01$. We also investigated how the strenght of the coupling between both baths affects the thermalization of the OQS in Fig. 9b. We kept all values constant, and only varied g_2, which reduces the decay rate of the OQS for bigger values. The case were g_2 is null represents model A. From this graphic and the previous one it can readily be seen that the OQS thermalizes slower in the presence of a second reservoir.

When the baths have different temperatures, the process of thermalization might be harder to achieve or even not possible, since the equilibrium between reservoirs might not be reached. In Fig. 10a we show a simulation where $\beta_1 < \beta_2$ and, in Fig. 10b, one with $\beta_1 > \beta_2$. We can speculate from this graphics that the bath that dominates the thermalization is the second reservoir. It would make sense, since each mode of the RI is like another OQS with its own environment, meaning that the RII would thermalize RI at the temperature β_2 and then the OQS would thermalize to a state with that inverse temperature. We emphasize that these results are not conclusive, and a more extensive study of the system should be conducted.

10 Conclusions and future perspectives

In this work, the theory of open quantum systems has been introduced along with the presentation of some canonical models and the charaterization of the environment. The evolution of OQS has been inspected, together with the concept of Markovianity. A perturbative method has been introduced to study the evolution of OQS, and then applied to a variety of situations. It is of special interest the case where the environment is coupled to a second reservoir. We have simulated different environments with a variety of parameters, upon which we base the following conclusions.

First of all, the ME derived in section 5 correctly describes de dynamics of the OQS in the weak coupling limit. The ME description of the dynamics is limited due to the fact that we trace out the environment, and no information about it is available, apart from the correlation functions. We checked that this ME does indeed represent well the evolution of the OQS by comparison with some models that have an anallytic solution.

We used the weak coupling ME to study the situation of a spin-$\frac{1}{2}$ system coupled to a bosonic bath, and explored how the properties of the environment affect the thermalization time scale. We found that, when the spectral density of the bath is wider, the thermalization occurs in shorter time scales. We also found that, when the temperature of the reservoir is higher, the OQS thermalizes faster, and that Ohmic reservoirs present slower thermalization decay rates.

The situation where the OQS is coupled to a reservoir that is in turn coupled to a second one has not been, to our knowledge, explored in the literature, and the concepts are not clear at first glance. We found that, in the case that both reservoirs have the same properties, the inclusion of a second reservoir causes a decrease in the thermalization rate of the OQS, and also that this decay is slower when the coupling between baths is stronger, but still inside the range of the weak coupling limit. This can be understood, in a qualitative way, by considering that the perturbation the OQS induces onto the RI are also transfered to the RII, meaning that now the two baths are outside equilibrium. The RI has to be in equilibrium so that the OQS can thermalize, and this equilibrium might be harder to achieve under the presence of a second reservoir, when the additional time scale of RII is present, which can delay the thermalization. In the case where the two baths are at different temperatures, the thermalization occours at a much larger time scale, as expected, since the equilibrium conditions of the reservoirs are harder to achieve.

The idea of introducing the second reservoir can be explored using different models. This work has the natural continuation in a doctoral thesis to develope this new idea and, for instance, by considering the configuration presented in Fig 11, where the OQS is coupled to the RI in a star configuration, and the RI is coupled to a common reservoir of harmonic oscillators RII. The Hamiltonian of the environment for this model is

$$H_E = \sum_{\lambda} \omega_\lambda a_\lambda^\dagger a_\lambda + \sum_k \omega_k b_k^\dagger b_k + \sum_{\lambda,k} \left(\tilde{g}_k a_\lambda b_k^\dagger + \tilde{g}_k^* a_\lambda^\dagger b_k \right) \,, \tag{153}$$

where b_k are the harmonic oscillators operators with frequency ω_k of RII and $\tilde{g}_k$ is the coupling strength constant between any mode of RI and the k-th oscillator of RII. These operators obey the commutation relation $[b_k, b_{k'}^\dagger] = \delta_{k,k'}$. It will be also very interesting to fully understant the process of thermalization from a wider point of view. A full study of the system should be performed to understand the equilibrium conditions that both

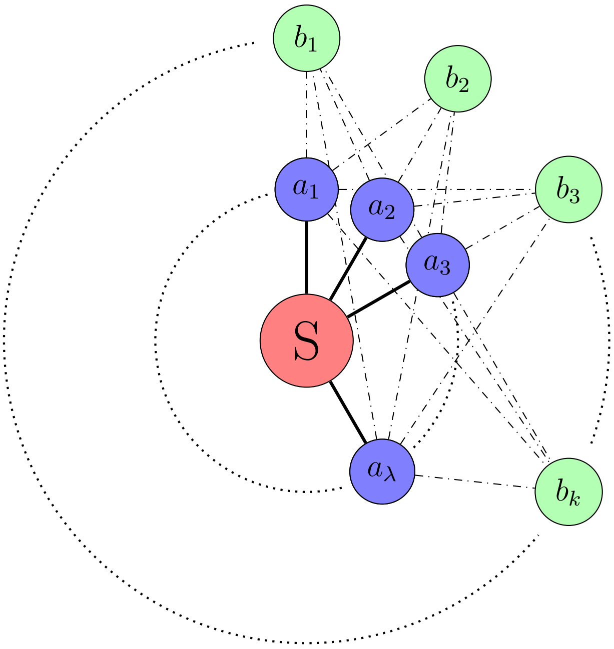


Figure 11: Schematic picture of Model C. The OQS is coupled, in a star configuration, to a set of harmonic oscillators a_λ, which are coupled to a common bath of harmonic oscillators b_k.

baths follow. There are techniques such as matrix product states [17] and tensor networks [18] that allow to study the full system, and trace out any subspace to focus, for instance, on what happens to the RI.

Appendices

A Weak coupling ME calculations

We left the more laborious calculations of section 5 to this appendix to allow for a fluent reading.

A.1 $\mathbf{Tr}_E\left[V_t H_I(t), \hat{\rho}(0)\right] = 0$ for an arbitrary state of the environment.

We have that $V_t^0 H_I = V_t L\ B^\dagger(t) + V_t L^\dagger\ B(t)$, and that the initial state of the system is uncorrelated, i.e., $\rho(0) = \rho_S(0)\rho_E(0)$. We now have

$$\begin{aligned}\mathrm{Tr}_E\left[V_t H_I(t), \hat{\rho}(0)\right] &= \mathrm{Tr}_E\left[V_t L\ B^\dagger(t) + V_t L^\dagger\ B(t), \rho_S(0)\rho_E(0)\right] = \\ &= \mathrm{Tr}_E\left[V_t L\ B^\dagger(t), \rho_S(0)\rho_E(0)\right] + \mathrm{Tr}_E\left[V_t L^\dagger\ B(t), \rho_S(0)\rho_E(0)\right]\ . \end{aligned} \tag{154}$$

If we focus on the first term (the result is similar for the second one),

$$\begin{aligned}\mathrm{Tr}_E\left[V_t L\ B^\dagger(t), \rho_S(0)\rho_E(0)\right] =& \mathrm{Tr}_E\{V_t L \rho_S(0) B^\dagger(t)\rho_E(0) - \rho_S(0) V_t L \rho_E(0) B^\dagger(t)\} = \\ =& \left[V_t L, \rho_S(0)\right] \mathrm{Tr}_E\{B^\dagger(t)\rho_E(0)\}\ , \end{aligned} \tag{155}$$

where the cyclic property of the trace has been used. Then the trace for a general state of the environment $\rho_E(0) = \sum_k p_k \left|k\right\rangle\left\langle k\right|$ is

$$\mathrm{Tr}_E\{B^\dagger(t)\rho_E(0)\} = \sum_{k,l} \langle l|B^\dagger(t)|k\rangle\, p_k\, \langle k|l\rangle\ , \tag{156}$$

where $\langle k|l\rangle = \delta_{kl}$ and

$$\langle l|B^\dagger(t)|k\rangle = \sum_\lambda g_\lambda^* \langle l|a_\lambda^\dagger|k\rangle = \sum_\lambda g_\lambda^* \delta_{l,k+1}\ , \tag{157}$$

which will lead to a null result of the trace since we have two deltas with mismatching indices inside the sumatory.

A.2 Computation of $\mathbf{Tr}_E\left[V_t^0 H_I(t), \left[V_\tau^0 H_I(\tau), \hat{\rho}(0)\right]\right]$

We first compute the commutator of the first term in the interaction Hamiltonian with the total density matrix

$$\left[V_\tau L^\dagger \otimes B(\tau), \rho_S(0)\otimes\rho_E(0)\right] = V_\tau L^\dagger \rho_S(0) \otimes B(\tau)\rho_E(0) - \rho_S(0) V_\tau L^\dagger \otimes \rho_E(0) B(\tau)\ , \tag{158}$$

and then operate the commutator of that with the second term of the interaction Hamiltonian, to end up with the trace of a B and a $B^\dagger$ operators, because, if we end up with the trace of two B or two $B^\dagger$ operators, the trace becomes null, in a similar fashion as in the previous section. With that in mind,

$$\begin{aligned}&\mathrm{Tr}_E\left[V_t L \otimes B^\dagger(t), \left[V_\tau L^\dagger \otimes B(\tau), \rho_S(0)\otimes\rho_E(0)\right]\right] = \\ &\qquad V_t L V_\tau L^\dagger \rho_S(0) \mathrm{Tr}_E\{B^\dagger(t) B(\tau)\rho_E(0)\} - V_t L \rho_S(0) V_\tau L^\dagger \mathrm{Tr}_E\{B^\dagger(t)\rho_E(0) B(\tau)\} - \\ &\qquad V_\tau L^\dagger \rho_S(0) V_t L \mathrm{Tr}_E\{B(\tau)\rho_E(0) B^\dagger(t)\} + \rho_S(0) V_\tau L^\dagger V_t L \mathrm{Tr}_E\{\rho_E(0) B(\tau) B^\dagger(t)\}\ . \end{aligned} \tag{159}$$

Making use of the cyclic property of the trace we can group the previous equation into two commutators

$$\begin{aligned}&\mathrm{Tr}_E\{B^\dagger(t)B(\tau)\rho_E(0)\}[V_tL, V_\tau L^\dagger\rho_S(0)]+\\&\mathrm{Tr}_E\{B(\tau)B^\dagger(t)\rho_E(0)\}[\rho_S(0)V_\tau, L^\dagger V_tL]\ ,\end{aligned} \tag{160}$$

To calculate the other non-null term of $\mathrm{Tr}_E\left[V_t^0H_I(t), [V_\tau^0H_I(\tau), \hat{\rho}(0)]\right]$ a similar procedure is followed to yield the final result

$$\begin{aligned}&\mathrm{Tr}_E\{B^\dagger(t)B(\tau)\rho_E(0)\}\left[V_tL, V_\tau L^\dagger\rho_S(0)\right] + \mathrm{Tr}_E\{B(\tau)B^\dagger(t)\rho_E(0)\}\left[\rho_S(0)V_\tau, L^\dagger V_tL\right] +\\&\mathrm{Tr}_E\{B(t)B^\dagger(\tau)\hat{\rho}_E(0)\}\left[V_tL^\dagger, V_\tau L\rho_S(0)\right] + \mathrm{Tr}_E\{B^\dagger(\tau)B(t)\rho_E(0)\}\left[\rho_S(0)V_\tau L^\dagger, V_tL\right]\ .\end{aligned} \tag{161}$$

A.3 Switching to the Schrödinger picture

The Schröndinger picture density matrix operator, in terms of the operator in the interaction picture, is

$$\rho_S(t) = e^{-iH_St}\hat{\rho}_S(t)e^{iH_St}\ , \tag{162}$$

and the derivative of this operator becomes

$$\frac{d}{dt}\rho_S(t) = (-iH_S)e^{-iH_St}\hat{\rho}_S(t)e^{iH_St} + e^{-iH_St}\hat{\rho}_S(t)e^{iH_St}(iH_S) + e^{-iH_St}\left(\frac{d}{dt}\hat{\rho}_S(t)\right)e^{iH_St}\ . \tag{163}$$

The first two terms can be gathered into the commutator $-i\left[H_S, \rho_S(t)\right]$, and the third one needs to be explicitly computed from Eq. (45). We will compute the action of these exponentials on the first commutator

$$\begin{aligned}e^{-iH_St}\left[V_\tau L^\dagger\hat{\rho}_S(t), V_tL\right]e^{iH_St} =&e^{-i\omega_0t}e^{i\omega_0\tau}L^\dagger e^{-i\omega_0\tau}e^{i\omega_0t}\rho_S(t)e^{-i\omega_0t}e^{i\omega_0t}Le^{-i\omega_0t}e^{i\omega_0t}-\\&e^{-i\omega_0t}e^{i\omega_0t}Le^{-i\omega_0t}e^{i\omega_0\tau}L^\dagger e^{-i\omega_0\tau}e^{i\omega_0t}\rho_S(t)e^{-i\omega_0t}e^{i\omega_0t}\end{aligned} \tag{164}$$

where direct cancellation of some exponentials and $e^{-i\omega_0t}e^{i\omega_0\tau}L^\dagger e^{-i\omega_0\tau}e^{i\omega_0t} = V_{\tau-t}L^\dagger$ lead to

$$V_{\tau-t}L^\dagger\rho_S(t)L - LV_{\tau-t}L^\dagger\rho_S(t) = \left[V_{\tau-t}L^\dagger\rho_S(t), L\right]\ . \tag{165}$$

The same procedure is followed to compute the remaining commutators in the Schrödinger picture.

B Commutators of weak coupling ME for different OQS operators L

We left the computation of the commutators appearing in the weak ME for different operators acting on the system to this appendix.

B.1 $L = \sigma_- \; (L^\dagger = \sigma_+)$

$$\left[V_{-m}L^\dagger\rho_S(t), L\right] = \begin{pmatrix} \rho_{--}(t)e^{-i\omega_0 m} & 0 \\ -\rho_{-+}(t)e^{-i\omega_0 m} & -\rho_{--}(t)e^{-i\omega_0 m} \end{pmatrix} \tag{166}$$

$$\left[L, \rho_S(t)V_{-m}L^\dagger\right] = \begin{pmatrix} -\rho_{++}(t)e^{-i\omega_0 m} & 0 \\ -\rho_{-+}(t)e^{-i\omega_0 m} & \rho_{++}(t)e^{-i\omega_0 m} \end{pmatrix} \tag{167}$$

$$\left[V_{-m}L\rho_S(t), L^\dagger\right] = \begin{pmatrix} -\rho_{++}(t)e^{i\omega_0 m} & -\rho_{+-}(t)e^{i\omega_0 m} \\ 0 & \rho_{++}(t)e^{i\omega_0 m} \end{pmatrix} \tag{168}$$

$$\left[L^\dagger, \rho_S(t)V_{-m}L\right] = \begin{pmatrix} \rho_{--}(t)e^{i\omega_0 m} & -\rho_{+-}(t)e^{i\omega_0 m} \\ 0 & -\rho_{--}(t)e^{i\omega_0 m} \end{pmatrix} \tag{169}$$

B.2 $L = L^\dagger = \sigma_z$

$$\left[V_{-m}L^\dagger\rho_S(t), L\right] = \left[V_{-m}L\rho_S(t), L^\dagger\right] = \begin{pmatrix} 0 & -2\rho_{+-}(t) \\ -2\rho_{-+}(t) & 0 \end{pmatrix} \tag{170}$$

$$\left[L^\dagger, \rho_S(t)V_{-m}L\right] = \left[L, \rho_S(t)V_{-m}L^\dagger\right] = \begin{pmatrix} 0 & -2\rho_{+-}(t) \\ -2\rho_{-+}(t) & 0 \end{pmatrix} \tag{171}$$

$$\tag{172}$$

B.3 $[H_S, \rho_S(t)]$

$$[H_S, \rho_S(t)] = \frac{\omega_0}{2}\begin{pmatrix} 0 & 2\rho_{+-}(t) \\ -2\rho_{-+}(t) & 0 \end{pmatrix} \tag{173}$$

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