Validity of the Lindblad Master Equations

Master’s thesis

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Abstract

Theory of open quantum systems, which studies quantum systems interacting with their environments, has a wide variety of applications in physics, ranging from quantum optics and condensed matter physics to quantum informatics and quantum computation. One important feature of open quantum systems is quantum mechanical treatment for damping, which is usually described by Lindblad master equations derived using the Born–Markov approximation. However, because of their perturbative nature, such master equations can only model systems with weak system-environment coupling. For example, in superconducting quantum circuits the environmental coupling can be increased to values for which the master equations are no longer accurate. A more accurate equation of motion, the formally exact stochastic Liouville–von Neumann equation, can be obtained by using the path integral formalism of quantum mechanics.

We study a simple but important model where a two state system, qubit, is coupled to a quantum harmonic oscillator, which is further coupled to a harmonic oscillator bath. The qubit-oscillator system can be described by the Rabi Hamiltonian. We solve the dynamics of this system numerically with the stochastic Liouville–von Neumann equation and two different Lindblad master equations, the quantum optical master equation and the eigenstate master equation. The former treats the qubit and the oscillator separately and the transitions occur between the eigenstates of the oscillator, whereas the latter treats them as a single system with transitions between the eigenstates of the whole system Hamiltonian. Numerical solutions of the stochastic Liouville–von Neumann equation are unstable with long simulation times. Because of this we are only able to solve it in the case where the qubit and the oscillator are in resonance. In this case we find parameters with which all three equations produce nearly the same results. We also see that there exists cases where only one of the master equations agrees with the stochastic Liouville–von Neumann equation. Furthermore, we find parameters for which both master equations produce results that deviate notably from those given by the stochastic Liouville–von Neumann equation. In off-resonance, we find that the solutions of the two master equations do not agree with each other for any parameters we study.

These results suggest that the current state of the numerical simulations of open quantum systems can be improved by using the formally exact methods instead of the approximate ones for situations where the environmental coupling is of the order of the qubit-cavity coupling or stronger.
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1. Introduction

Theory of open quantum systems describes the behaviour of quantum systems interacting with their surroundings [1]. One important application is the quantum mechanical treatment for dissipation and damping [2]. In quantum mechanics the time evolution is produced by the Hamiltonian operator. Problem with this is that the generated dynamics conserves energy, which makes it difficult to model dissipative processes in closed quantum systems. However, if one instead considers a situation where the studied quantum system is interacting with some environment containing large number of degrees of freedom, the energy can be transferred from the system to the environment. From the system point of view this is seen as dissipation, even though the total energy of the system and the environment is conserved. Properties of the studied quantum system can be described by the reduced density operator, which contains all the measurable information of the system [3, 4]. It is therefore important to have an equation of motion for the reduced density operator. Because of the large number of degrees of freedom, it is often impossible to solve these equations analytically. Even though one can obtain exact results numerically by using the path integral formalism, this is usually extremely cumbersome. If one makes few simple assumptions about the environment, one can derive the formally exact stochastic Liouville–von Neumann equation, which then governs the time evolution of the reduced density operator [5, 6, 7, 8, 9, 10]. The dissipation in this equation is produced by two stochastic complex valued noise terms. Usually in the literature the dynamics of open quantum systems are not solved exactly. Instead, if the coupling between the studied system and the environment is weak, one can make several approximations and obtain master equations in the Lindblad form [11, 12, 13].

The simplest quantum mechanical system is the two-state system, which is often referred to as quantum bit or just qubit. Another important system is the quantum harmonic oscillator. The Rabi Hamiltonian describes a system where these two systems are coupled [14, 15]. If the coupling energy between the qubit and the oscillator is much weaker than the uncoupled energies and if the qubit and the oscillator are near resonance, one can make the rotating wave approximation and obtain the Jaynes–Cummings Hamiltonian [16, 17]. An open quantum system consisting of the qubit-oscillator system where the oscillator is further interacting with the environment has many applications in a wide variety of fields of physics. In quantum optics and cavity quantum electrodynamics it describes the radiation-matter interaction, for example a two state atom interacting with a photon in a cavity, which is a narrow mirror system where photons can be trapped [14, 15]. In circuit quantum electrodynamics it is used for modeling the coupling between artificial atoms, such as superconducting Cooper pair boxes, and transmission line resonators or LC circuits [18, 19]. One of the most active fields of research at the moment is quantum computation and quantum information. In a classical computer the computation is based on bits, which can have a value 0 or 1. In quantum computer the computation can in principle be done using quantum bits, qubits, which can be in any linear combination of 0 and 1 states. In order to use quantum computer one has to initialize its qubits into well-defined initial states. This can be done for example with qubit-resonator-reservoir components, a quantum system that can be described by the qubit-oscillator system interacting with the environment [20, 21, 22, 23].

In the above mentioned cases the dynamics of the qubit-oscillator system are usually solved by using the Lindblad master equations. In quantum optical systems the qubit-oscillator coupling is so weak that the Jaynes–Cummings Hamiltonian can be used as an approximation [24]. Because of this one often derives the master equation with the assumption that the qubit and the cavity are not coupled [25, 26, 27, 28]. Resulting master equation therefore contains dissipators that induce transitions between the eigenstates of the cavity. The interaction between the qubit and the cavity is added later on. This master equation thus effectively treats the qubit and the cavity as separate systems. This model agrees well with the experiments performed on the quantum optical systems. In circuit quantum electrodynamics and quantum computers, however, the coupling between the qubit and the oscillator can be so strong that the Jaynes–Cummings model is no longer valid [14, 18, 29]. Because of this, the master equation used in quantum optics is not valid. Fortunately, one can derive a master equation which treats the qubit-oscillator system as a single system, thus inducing transitions between the eigenstates of the system Hamiltonian [4, 11, 12]. If the environmental coupling is strong enough, the master equation approach to system dynamics is no longer accurate. In such cases one has to resort to the exact methods by using, for example, the stochastic Liouville–von Neumann equation.

The aim of this thesis is to solve numerically the two master equations and the stochastic Liouville–von Neumann equation for the qubit-cavity system and find the parameter regions where the exact solution can be approximated by the master equations. As far as we know, this computation has not been performed previously for the qubit-cavity system. The knowledge about the differences between the solutions of the exact stochastic Liouville–von Neumann equation and the approximate master equations is important. For example, if one models the components of the quantum computer with a master equation, the model might be too inaccurate to produce realistic results.
This thesis proceeds as follows. In Section 2, we introduce some key features of composite quantum systems. We then apply these and present the concept of open quantum systems. We also discuss four different ways of treating time dependence in quantum mechanics, namely Schrödinger, Heisenberg and interaction pictures and Feynman path integrals. In Section 3, we define the Hamiltonian of our system, namely the Rabi Hamiltonian. We perform the rotating wave approximation and obtain the Jaynes–Cummings Hamiltonian. We present analytical solutions for the eigenproblem of the Jaynes–Cummings Hamiltonian, and use the second order perturbation theory for the Rabi Hamiltonian. We model the environment with a bosonic bath in thermal equilibrium and discuss its properties. In Section 4, we present three different equations governing the time evolution of the system density operator, namely the two different Lindblad master equations and the stochastic Liouville–von Neumann equation. A thorough derivation of the master equations is given and the differences between the two are discussed. After this the stochastic Liouville–von Neumann equation is derived. We also calculate the proper window functions needed for the generation of the stochastic complex noises. We end the section with a discussion about the equilibrium solutions of the equations. The numerical methods we used are described in Section 5 together with the discussion about the simulation parameters. The numerical results are given in Section 6. Section 7 is reserved for the conclusions.


2. Quantum mechanical background

2.1. Composite and open quantum systems

Let us begin by introducing the concept of composite quantum systems. Consider a system that can be separated into two individual components. Let the individual Hilbert spaces be $\mathcal{H}_1$ and $\mathcal{H}_2$, and let the vectors in these spaces be denoted with

$$|\alpha_1\rangle \in \mathcal{H}_1, \quad |\beta_2\rangle \in \mathcal{H}_2.$$  \hspace{1cm} (2.1)

The Hilbert space of the composite system consisting of vectors in spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ can be written as $[1, 3, 30]

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2.$$  \hspace{1cm} (2.2)

Vectors in this space can then be written as

$$|\alpha_1, \beta_2\rangle = |\alpha_1\rangle \otimes |\beta_2\rangle.$$  \hspace{1cm} (2.3)

The symbol $\otimes$ is known as the tensor or Kronecker product. Inner products in $\mathcal{H}$ can be calculated as

$$\langle \alpha'_1, \beta'_2 | \alpha_1, \beta_2 \rangle = \langle \alpha'_1 | \alpha_1 \rangle \langle \beta'_2 | \beta_2 \rangle.$$  \hspace{1cm} (2.4)

Operators that act on spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ must act similarly also in $\mathcal{H}$. We can therefore define the product space operators as Kronecker products:

$$(\hat{A}_1 \otimes \hat{A}_2) |\alpha_1, \beta_2\rangle = (\hat{A}_1 |\alpha_1\rangle) \otimes (\hat{A}_2 |\beta_2\rangle).$$  \hspace{1cm} (2.5)

If we have an operator that only acts in one of the subspaces, we can write it as a Kronecker product with the identity operator $I$, e.g.

$$(\hat{A}_1 \otimes I) |\alpha_1, \beta_2\rangle = (\hat{A}_1 |\alpha_1\rangle) \otimes |\beta_2\rangle.$$  \hspace{1cm} (2.6)

If vectors $|a_{1n}\rangle$ and $|a_{2m}\rangle$, $n = 1, 2, \ldots$ form the bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, then a basis of $\mathcal{H}$ can be expressed as

$$\{|a_{1n}, a_{2m}\rangle\} = \{|a_{1n}\rangle \otimes |a_{2m}\rangle\}, \quad n, m = 1, 2, \ldots$$  \hspace{1cm} (2.7)

Matrix elements of the operator $\hat{A}_1 \otimes \hat{A}_2$ can be written as $[1, 3, 30]

$$\langle a'_{1n}, a'_{2m} | \hat{A}_1 \otimes \hat{A}_2 | a_{1n}, a_{2m}\rangle = \langle a'_{1n} | \hat{A}_1 | a_{1n}\rangle \langle a'_{2m} | \hat{A}_2 | a_{2m}\rangle.$$  \hspace{1cm} (2.8)

Closed quantum systems are quantum mechanical systems that are not interacting with their environments. A textbook example of such system is a particle in an infinite potential well. In reality, however, closed quantum system cannot exist, since the interaction with the outside world cannot be removed completely [1]. All quantum mechanical systems that can be found in nature are therefore open quantum systems. Their Hamiltonian can be written as

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I,$$  \hspace{1cm} (2.9)

where $\hat{H}_S$ is the Hamiltonian of the studied quantum system, $\hat{H}_B$ is the Hamiltonian of the environment and $\hat{H}_I$ describes the interaction between the studied system and the environment. Usually the quantum system under study is much smaller than the environment. It is therefore often referred to as small quantum system. System described by the Hamiltonian (2.9) is an example of a composite quantum system, where we interpret the studied system as system 1 and the environment as system 2 in previous notation. The Hilbert space of the open quantum system can therefore be written as a Kronecker product of the Hilbert spaces of the studied system and the environment:

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B.$$  \hspace{1cm} (2.10)

This way we can express Eq. (2.9) as

$$\hat{H} = \hat{H}_S \otimes \hat{I}_B + \hat{I}_S \otimes \hat{H}_B + \hat{H}_I,$$  \hspace{1cm} (2.11)

where $\hat{I}_S$ and $\hat{I}_B$ are identity operators with dimensions of the environment and the studied system, respectively. If the environment has an infinite number of degrees of freedom, it is referred to as a reservoir. Further, if the reservoir is in the thermal equilibrium, it is called a heat bath or just a bath. [1]
Density operator of a quantum system is defined as \[ \hat{\rho} = \sum_n \sum_m \rho_{nm} |\psi_n\rangle \langle \psi_m|, \] (2.12)

where \(|\psi_n\rangle\) is a set of basis states. This operator is Hermitian. Sometimes it is written in a diagonal basis, where it has the form

\[ \hat{\rho} = \sum_n \rho_n |\psi_n\rangle \langle \psi_n|, \] (2.13)

where \(\rho_n\) is the occupation probability of the state \(|\psi_n\rangle\). All probabilities \(\rho_n\) have to be positive real numbers and their sum must be unity, i.e.

\[ \text{Tr} \hat{\rho} = 1. \] (2.14)

All measurable information of the system is contained in the density operator [1, 32], since the expectation value of any observable \(\hat{A}\) can be obtained by calculating

\[ \langle \hat{A} \rangle = \text{Tr}[\hat{A} \hat{\rho}]. \] (2.15)

In the case of open quantum systems we are usually interested only in the studied system observables \(\hat{A}_S\). Their expectation values are determined by [1, 2, 3, 4, 30]

\[ \langle \hat{A}_S \rangle = \text{Tr}[\hat{A}_S \hat{\rho}_S], \] (2.16)

where \(\hat{\rho}_S\) is the density operator of the studied system, which is often referred to as reduced density operator. It can be obtained from the density operator of the total system by tracing out the environmental degrees of freedom [1, 2, 4, 31]:

\[ \hat{\rho}_S = \text{Tr}_B \hat{\rho}. \] (2.17)

### 2.2. Representations of quantum mechanics

Let us then briefly discuss different ways of treating time dependence in quantum mechanics. In elementary quantum mechanics courses one learns that the time evolution of a quantum state is fully governed by the Schrödinger equation, and it is the state vector that is evolving in time. This is called the Schrödinger picture. Closer resemblance with the classical mechanics can be obtained in the Heisenberg picture, where it is the operators that change in time, not the states. These two are limiting cases of the interaction or Dirac picture, where some of the time dependence is contained in the state vectors and some in the operators. Quantum mechanics can also be formulated with path integrals.

#### 2.2.1. Three pictures

In the Schrödinger picture the operators are time-independent (they can depend on time explicitly, though). Time dependence is fully included in the state vectors (density operator) [1, 2, 3, 30]. Thus, we can consider a system that at some arbitrary time \(t_0\) is in state \(|\psi(t_0)\rangle\). At some later time \(t\), the system is then expressed as \(|\psi(t,t_0)\rangle\). The time evolution is obtained from the Schrödinger equation

\[ i\hbar \frac{\partial |\psi(t,t_0)\rangle}{\partial t} = \hat{H}(t) |\psi(t,t_0)\rangle, \] (2.18)

where \(\hat{H}(t)\) is the Hamiltonian of the system. Solution of the Schrödinger equation can be written with the unitary time-evolution operator \(\hat{U}(t,t_0)\), defined as:

\[ |\psi(t,t_0)\rangle = \hat{U}(t,t_0) |\psi(t_0,t_0)\rangle. \] (2.19)

By substituting this expression into the Schrödinger equation (2.18), we obtain an equation of motion for the time-evolution operator

\[ i\hbar \frac{\partial \hat{U}(t,t_0)}{\partial t} = \hat{H}(t) \hat{U}(t,t_0), \] (2.20)

with an initial condition

\[ \hat{U}(t_0,t_0) = \hat{I}. \] (2.21)
If the Hamiltonian is time-independent, the solution of Eq. (2.20) is trivial:

$$\hat{U}(t, t_0) = \exp \left[ -\frac{i}{\hbar} \hat{H}(t - t_0) \right] . \quad (2.22)$$

Using the time-evolution operator, we can obtain a dynamical equation for the density operator. In the Schrödinger picture, the time dependence is contained in the state vectors, so we can write the time dependence of the density operator (2.13) explicitly as

$$\dot{\hat{\rho}}(t) = \sum_n \rho_{nn} \langle \psi_n; t, t_0 \rangle \langle \psi_n; t_0, t \rangle = \sum_n \rho_{nn} \hat{U}(t, t_0) \langle \psi_n; t_0, t \rangle \langle \psi_n; t_0, t \rangle \hat{U}^\dagger(t, t_0)$$

$$= U(t, t_0) \hat{\rho}(t_0) U^\dagger(t, t_0). \quad (2.23)$$

By differentiating this with respect to time and using Eq. (2.20) we obtain an equation for the time evolution of the density operator:

$$i\hbar \frac{d\hat{\rho}(t)}{dt} = [\hat{H}(t), \hat{\rho}(t)]. \quad (2.24)$$

This is the von Neumann or Liouville–von Neumann equation. [1, 2, 3, 25, 30, 31]

However, instead of assuming that the time dependence is in the state vectors, we can assume that the state vectors are constants in time and the time dependence is included in the operators. This representation is called the Heisenberg picture [1, 2, 3, 30]. Let us assume that at some arbitrary time \(t_0\) the states are the same in both pictures, i.e. \(\hat{\rho}(t_0) = \hat{\rho}_H(t_0)\), where subscript \(H\) stands for Heisenberg. We can obtain an arbitrary Heisenberg picture operator \(\hat{A}_H\) from the corresponding operator in the Schrödinger picture \(\hat{A}\) by the canonical transformation:

$$\hat{A}_H(t) = U^\dagger(t, t_0) \hat{A}(t) U(t, t_0), \quad (2.25)$$

where explicit time dependence in the Schrödinger picture operator is allowed. The time evolution of the operator \(\hat{A}_H\) is governed by the equation [1, 2, 3, 30]

$$i\hbar \frac{d\hat{A}_H}{dt} = [\hat{A}_H, \hat{H}_H] + i\hbar \frac{\partial \hat{A}_H}{\partial t}. \quad (2.26)$$

where

$$\frac{\partial \hat{A}_H}{\partial t} = U^\dagger(t, t_0) \frac{\partial \hat{A}}{\partial t} U(t, t_0). \quad (2.27)$$

Third way of considering the time evolution is called the interaction picture [1, 2, 3, 30], which is sometimes referred to as Dirac picture [33]. Let us write the Hamiltonian in two parts,

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_I(t). \quad (2.28)$$

Here the time evolution is governed by an unitary time-evolution operator \(\hat{U}_0(t, t_0)\), which is defined so that

$$i\hbar \frac{d}{dt} \hat{U}_0(t, t_0) = \hat{H}_0 \hat{U}_0(t, t_0). \quad (2.29)$$

If \(\hat{H}_0\) is time-independent, time-evolution operator is simply

$$\hat{U}_0(t, t_0) = \exp \left[ -\frac{\hbar}{i} \hat{H}_0(t - t_0) \right]. \quad (2.30)$$

With these we can write the operators in the interaction picture as

$$\hat{A}_I(t) = \hat{U}_0^\dagger(t, t_0) \hat{A}(t) \hat{U}_0(t, t_0), \quad (2.31)$$

$$\hat{\rho}_I(t) = \hat{U}_0^\dagger(t, t_0) \hat{\rho}(t) \hat{U}_0(t, t_0). \quad (2.32)$$

If we set \(\hat{H}_I(t) = 0\), we obtain the Schrödinger picture, and if we set \(\hat{H}_0 = 0\), we obtain the Heisenberg picture. Therefore one can say that the interaction picture is more general than Schrödinger and Heisenberg pictures. [1, 3]

We now have three ways of writing the time-dependence in quantum mechanics. However, this must not affect the way we observe quantum mechanical phenomena. It turns out that the time-dependence of the expectation values of the observables is independent on the picture we are using, i.e. \(\frac{d}{dt} \langle \hat{A}(t) \rangle = \frac{d}{dt} \langle \hat{A}_I(t) \rangle = \frac{d}{dt} \langle \hat{A}_H(t) \rangle \). Thus, it
We can write the product of the operators in the left hand side of Eq. (2.34) as

\[ H = \frac{d}{dt} U_0(t) \frac{d}{dt} \hat{\rho} U_0(t) = \frac{d}{dt} \left( U_0(t) \hat{\rho} U_0(t)^\dagger \right) \]

where in the second line we have used the fact that \( \hat{U}_0 \) and \( \hat{\rho} \) are the eigenvalues of the position and momentum operators, respectively.

By using Eq. (2.29), we can write Eq. (2.37) as

\[ \frac{d}{dt} \hat{U}_0(t) \hat{\rho} \hat{U}_0(t)^\dagger = \frac{d}{dt} \left( \hat{U}_0(t) \hat{\rho} \hat{U}_0(t)^\dagger \right) \]

where in the second line we have used the path integral formalism by R. Feynman. Before going to that, we first state few properties of the position and momentum observables in quantum mechanics. Let us denote the eigenstates of the position and momentum operators as \( \hat{q} \) and \( \hat{p} \) as \( |q\rangle \) and \( |p\rangle \), respectively:

\[ \hat{q} |q\rangle = q |q\rangle, \quad \hat{p} |p\rangle = p |p\rangle \]

where \( q \) and \( p \) are the eigenvalues of the position and momentum operators, respectively. These states are normalized in terms of the Dirac delta function as

\[ \langle q | q' \rangle = \delta(q - q'), \quad \langle p | p' \rangle = \delta(p - p') \]

and they form a complete basis, which allows us to write the identity operator as

\[ I = \int_{-\infty}^{\infty} dq |q\rangle \langle q| = \int_{-\infty}^{\infty} dp |p\rangle \langle p| \]

Further, they obey relation [3, 30, 34]

\[ \langle q | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{iqp/\hbar}. \]

Let us then consider a simple quantum point particle whose initial state at time \( t = 0 \) is \( |q_i\rangle \). The amplitude for the particle to propagate from this state to state \( |q_f\rangle \) in time \( t \) is governed by the unitary time evolution operator (2.22) as [3, 5, 34]

\[ \langle q_f | \hat{U}(t, 0) | q_i \rangle = \langle q_f | e^{-i\hat{H}t/\hbar} | q_i \rangle. \]
If we divide the time \( t \) into \( N \) short time intervals \( \delta t = t/N \), we obtain
\[
\langle q_t | e^{-i\hat{H}t/\hbar} | q_i \rangle = \langle q_t | e^{-i\hat{H}\delta t/\hbar} e^{-i\hat{H}\delta t/\hbar} \cdots e^{-i\hat{H}\delta t/\hbar} | q_i \rangle. \tag{2.48}
\]

Now, we insert the identity operator (2.45) between all exponentials in Eq. (2.48), which results in
\[
\langle q_t | e^{-i\hat{H}\delta t/\hbar} | q_i \rangle = \left( \prod_{j=1}^{N-1} \int dq_j \right) \langle q_i | e^{-i\hat{H}\delta t/\hbar} | q_{N-1} \rangle \langle q_{N-1} | e^{-i\hat{H}\delta t/\hbar} | q_{N-2} \rangle \cdots \langle q_1 | e^{-i\hat{H}\delta t/\hbar} | q_i \rangle. \tag{2.49}
\]

Let us then study an arbitrary inner product \( \langle q_{j+1} | e^{-i\hat{H}\delta t/\hbar} | q_j \rangle \). We assume that the Hamiltonian can be written as \( \hat{H} = \hat{p}^2/(2m) + V(\hat{q}) \), where \( m \) is the mass of the particle under study and \( V(\hat{q}) \) is the potential energy. We assume that \( \delta t \ll 1 \), so we can write
\[
\exp \left\{ -i\delta t \left[ \hat{p}^2 \over 2m + V(\hat{q}) \right] \right\} \approx \exp \left\{ -i\delta t \hat{p}^2 \over 2m \right\} \exp \left\{ -i\delta t V(\hat{q}) \right\}, \tag{2.50}
\]
which holds up to first order in \( \delta t \). Thus, we obtain
\[
\langle q_{j+1} | e^{-i\hat{H}\delta t/\hbar} | q_j \rangle = \langle q_{j+1} | \exp \left\{ -i\delta t \left[ \hat{p}^2 \over 2m + V(\hat{q}) \right] \right\} | q_j \rangle = \exp \left\{ -i\delta t V(q_j) \right\} \langle q_{j+1} | \exp \left\{ -i\delta t \hat{p}^2 \over 2m \right\} | q_j \rangle, \tag{2.51}
\]
where the potential energy is no longer an operator, since the position operators contained in it have operated on the position eigenstate \( |q_j\rangle \). In order to eliminate also the momentum operator, let us again use the identity operator, this time represented in the momentum space. We obtain
\[
\langle q_{j+1} | e^{-i\hat{H}\delta t/\hbar} | q_j \rangle = \exp \left\{ -i\delta t V(q_j) \right\} \int_{-\infty}^{\infty} dp \langle q_{j+1} | \exp \left\{ -i\delta t \hat{p}^2 \over 2m \right\} | p \rangle \langle p | q_j \rangle, \tag{2.52}
\]
\[
= \exp \left\{ -i\delta t V(q_j) \right\} \int_{-\infty}^{\infty} dp \exp \left\{ -i\delta t \hat{p}^2 \over 2m \right\} \langle q_{j+1} | p \rangle \langle p | q_j \rangle, \tag{2.53}
\]
\[
= \frac{1}{2\pi\hbar} \exp \left\{ -i\delta t V(q_j) \right\} \int_{-\infty}^{\infty} dp \exp \left\{ -i\delta t \hat{p}^2 \over 2m + i\hbar (q_{j+1} - q_j) \right\}, \tag{2.54}
\]
where in the second line the momentum operator has operated on the momentum eigenstate \( |p\rangle \) and in the third line we have used the relation (2.46). This integral can be solved by using
\[
\int_{-\infty}^{\infty} dx e^{-ax^2+bx} = e^{b^2/4a} \sqrt{\pi/a}, \tag{2.55}
\]
which can be verified by completing the square in the exponent. We obtain
\[
\langle q_{j+1} | e^{-i\hat{H}\delta t/\hbar} | q_j \rangle = \sqrt{-im \over 2\pi\hbar \delta t} \exp \left\{ i\delta t \left[ m(q_{j+1} - q_j)^2 \over 2\delta t^2 - V(q_j) \right] \right\}. \tag{2.56}
\]

With this, Eq. (2.49) can be written as
\[
\langle q_t | e^{-i\hat{H}t/\hbar} | q_i \rangle = \left( \frac{-im}{2\pi\hbar \delta t} \right)^{N/2} \left( \prod_{k=1}^{N-1} \int dq_k \right) \exp \left\{ i \sum_{j=0}^{N-1} \delta t \left[ m(q_{j+1} - q_j)^2 \over 2\delta t^2 - V(q_j) \right] \right\}. \tag{2.57}
\]

If we now go to the continuum limit by letting \( N \to \infty \) and \( \delta t \to 0 \), we replace \( (q_{j+1} - q_j)/\delta t \) by time derivative \( \dot{q} \) and sum \( \sum_{j=0}^{N-1} \delta t \) by integral \( \int_0^t dt' \). We also define the integral over all paths as \([5, 34]\)
\[
\int D[q] \equiv \lim_{N \to \infty} \left( \frac{-im}{2\pi\hbar \delta t} \right)^{N/2} \left( \prod_{k=1}^{N-1} \int dq_k \right).
\tag{2.58}
\]
We then obtain
\[
\langle q_t | e^{-i\hat{H}t/\hbar} | q_i \rangle = \int D[q] \exp \left\{ i \int_0^t dt' \left[ m \dot{q}^2 - V(q) \right] \right\}. \tag{2.59}
\]
The integrand in the exponent is just the classical Lagrangian of the particle, \( L(q, \dot{q}) \). Thus, we can identify the integral in the exponent as the classical action functional \( S[q] \) and write Eq. (2.59) as

\[
\langle q_f | e^{-i\hat{H}t/\hbar} | q_i \rangle = \int D[q] e^{i\hat{S}[q]}.
\] (2.60)

This is the Feynman’s path integral [3, 5, 34]. It is the probability amplitude for the particle to propagate from the state \( |q_i\rangle \) to the state \( |q_f\rangle \), and it is given by adding together the contributions of all possible paths. Contribution of a path is governed by \( \exp \{ \frac{i}{\hbar} S[q] \} \). In terms of the Schrödinger wave mechanics, we can identify the path integral (2.60) as the propagator \( G(q_f, q_i; t) \) [3]:

\[
G(q_f, q_i; t) = \int D[q] e^{i\hat{S}[q]}.
\] (2.61)

One can obtain the wave function of the system at time \( t \) with the propagator and the initial wave function as [3]

\[
\psi(q_f; t) = \int dq_i G(q_f, q_i; t) \psi(q_i).
\] (2.62)

Thus, the path integral formalism is just another way of solving the Schrödinger equation with some initial condition.

For an open quantum system we can generalize the path integral Eq. (2.60) as

\[
\langle q_f, \{q_n\} | e^{-i\hat{H}t/\hbar} | q_i, \{q_{n,i}\} \rangle = \int D[q] \int D^n[q_n] \exp \left\{ \frac{i}{\hbar} \left( S_S[q] + S_B[\{q_n\}] + S_I[\{q, \{q_n\}] \right) \right\},
\] (2.63)

where \( q \) is the system coordinate and \( \{q_n\} \) are the environmental coordinates, \( S_S[q] \), \( S_B[\{q_n\}] \) and \( S_I[\{q, \{q_n\}] \) are the classical action functionals corresponding to the system under study, its environment and their interaction, respectively [5].
3. System

Let us next define the system we study and its environment. Since the studied system is much smaller than the environment, from now on we refer to it as the small system.

3.1. Small system

We begin with the small system, where a qubit is coupled to a cavity. The Hamiltonian of the qubit is defined as

$$\hat{H}_Q = \hbar \omega_0 \hat{\sigma}_+ \hat{\sigma}_-,$$

where $\omega_0$ is the angular frequency, and $\hat{\sigma}_+$ and $\hat{\sigma}_-$ are the creation and annihilation operators of the qubit. The Hilbert space of the qubit is two dimensional with the basis states $|\downarrow\rangle$ and $|\uparrow\rangle$. The creation and annihilation operators act on them as [35]

$$\hat{\sigma}_+ |\downarrow\rangle = |\uparrow\rangle, \quad \hat{\sigma}_+ |\uparrow\rangle = 0, \quad \hat{\sigma}_- |\downarrow\rangle = 0, \quad \hat{\sigma}_- |\uparrow\rangle = |\downarrow\rangle.$$

Therefore, they are the eigenstates of the qubit Hamiltonian:

$$\hat{H}_Q |\downarrow\rangle = 0 |\downarrow\rangle,$$

$$\hat{H}_Q |\uparrow\rangle = \hbar \omega_0 |\uparrow\rangle$$

with the eigenvalues 0 and $\hbar \omega_0$, respectively. The cavity can be modelled with a simple quantum harmonic oscillator. Hamiltonian for it can be written as [3, 35]

$$\hat{H}_C = \hbar \omega_c \hat{a}^\dagger \hat{a},$$

where $\omega_c$ is the angular frequency and $\hat{a}^\dagger$ and $\hat{a}$ are the creation and annihilation operators of the harmonic oscillator. Note that we neglect the zero-point energy. The Hilbert space of the harmonic oscillator is infinite dimensional with the basis states $|n\rangle$, where $n = 0, 1, 2, \ldots$. The creation and annihilation operators act on these states as [3, 35]

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle, \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle.$$

Therefore, they are the eigenstates of the harmonic oscillator Hamiltonian with the eigenvalues $\hbar n \omega_c$:

$$\hat{H}_C |n\rangle = \hbar n \omega_c |n\rangle.$$  

The interaction between the qubit and the cavity is assumed to be bilinear and can therefore be written as

$$\hat{H}_{\text{int}} = \hbar g (\hat{a}^\dagger \hat{a} + \hat{\sigma}_+ \hat{\sigma}_-),$$

where $g$ is a parameter describing the strength of the interaction, usually referred to as the coupling. The Hamiltonian of the qubit-cavity system can then be written as

$$\hat{H}_R = \hat{H}_C + \hat{H}_Q + \hat{H}_{\text{int}}$$

$$= \hbar \omega_c (\hat{a}^\dagger \hat{a}) \otimes \hat{I}_Q + \hbar \omega_0 \hat{I}_C \otimes (\hat{\sigma}_+ \hat{\sigma}_-) + \hbar g (\hat{a}^\dagger \hat{a} + \hat{\sigma}_+ \hat{\sigma}_-)$$

$$= \hbar \omega_c \hat{a}^\dagger \hat{a} + \hbar \omega_0 \hat{\sigma}_+ \hat{\sigma}_- + \hbar g (\hat{a}^\dagger \hat{a} + \hat{\sigma}_+ \hat{\sigma}_-)$$

where on the third line we no longer write the Kronecker products explicitly. This is known as the Rabi Hamiltonian [14, 15, 18, 24, 29, 36, 37]. Even though there exists numerical proofs that it has a solution which can be presented in terms of elementary functions [36, 37], in practice one has to resort to purely numerical solutions of its eigenproblem. This Hamiltonian is sometimes falsely considered unphysical since terms $\hat{a}^\dagger \hat{\sigma}_+$ and $\hat{a} \hat{\sigma}_-$ do not conserve the total number of quanta in the system, which is described by the operator [14, 24]

$$\hat{N} = \hat{a}^\dagger \hat{a} + \hat{\sigma}_+ \hat{\sigma}_-.$$  

Nevertheless, these terms do not violate the conservation of energy since they do not affect the total energy of the system [24], which can be verified with the Heisenberg equation of motion (2.26)

$$i \hbar \frac{d\hat{H}_R}{dt} = [\hat{H}_R, \hat{H}_R] + \frac{\partial \hat{H}_R}{\partial t} = 0.$$
if the Hamiltonian is time-independent. Usually one performs the rotating wave approximation (RWA) to the interaction part of the Hamiltonian (3.11) to obtain an approximate Hamiltonian, which is analytically solvable. Let us derive that here. We assume that $g \ll \omega_q, \omega_c$, so that we can write operators in the interaction picture as

\[
\hat{a}_\downarrow(t) \approx \hat{a} e^{-i\delta t}, \quad (3.14)
\]
\[
\hat{a}_\uparrow(t) \approx \hat{a}^\dagger e^{i\delta t}, \quad (3.15)
\]
\[
\hat{\sigma}_-(t) \approx \hat{\sigma}_- e^{-i\delta t}, \quad (3.16)
\]
\[
\hat{\sigma}_+(t) \approx \hat{\sigma}_+ e^{i\delta t}. \quad (3.17)
\]

With these we can write the Hamiltonian in the interaction picture as

\[
\hat{H}_I(t) \approx \hbar g \left( \hat{a}^\dagger e^{i\omega_c t} + \hat{a} e^{-i\omega_c t} \right) \left( \hat{\sigma}_+ e^{i\omega_q t} + \hat{\sigma}_- e^{-i\omega_q t} \right),
\]
\[
= \hbar g \left( \hat{a}^\dagger \hat{\sigma}_+ e^{i(\omega_c + \omega_q) t} + \hat{a} \hat{\sigma}_- e^{i(\omega_c - \omega_q) t} + \hat{a} \hat{\sigma}_+ e^{-i(\omega_c - \omega_q) t} + \hat{a}^\dagger \hat{\sigma}_- e^{-i(\omega_c + \omega_q) t} \right),
\]
\[
\approx \hbar g \left( \hat{a}^\dagger \hat{\sigma}_+ e^{2i\omega t} + \hat{a} \hat{\sigma}_- + \hat{a} \hat{\sigma}_+ + \hat{a}^\dagger \hat{\sigma}_- e^{-2i\omega t} \right),
\]

where on the third line we assumed that the qubit and the cavity are near resonance ($\omega_c \approx \omega_q \equiv \omega$). We now notice that out of the four terms in (3.20), only two are time dependent, and further that they are oscillating with angular frequency $\pm 2\omega$. By claiming that these oscillations average out after a sufficiently long times ($t > 1/\omega$), we can neglect them. This procedure is the rotating wave approximation [2, 25, 27]. We are then left with the Hamiltonian (in the Schrödinger picture):

\[
\hat{H}_{JC} = \hbar \omega_q \hat{a}^\dagger \hat{a} + \hbar \omega_c \hat{\sigma}_+ \hat{\sigma}_- + \hbar g \left( \hat{a}^\dagger \hat{\sigma}_+ + \hat{a} \hat{\sigma}_- \right).
\]

This is known as the Jaynes–Cummings (JC) Hamiltonian, and it has been widely used in the literature in quantum optics, solid state physics, quantum information and quantum computations [2, 11, 12, 14, 15, 16, 17, 18, 19, 24, 28, 29, 38, 39, 40].

The approximation is valid if the coupling energy between the qubit and the cavity is small compared to the sum of the qubit and cavity energies i.e. $g \ll \omega_q, \omega_c$, and the qubit and the cavity are close to resonance, i.e. $\omega_q \approx \omega_c$ [11, 12, 15, 17, 24, 40]. The breakdown of the Jaynes–Cummings model has been verified also experimentally with sufficiently large coupling [18].

Let us then discuss the eigenvalues and eigenstates of the Jaynes–Cummings and Rabi Hamiltonians. We start by writing the basis vectors of the qubit-cavity system as a Kroenecker product of the qubit and harmonic oscillator basis vectors:

\[
|\downarrow n\rangle = |\downarrow\rangle \otimes |n\rangle,
\]

where $|\downarrow\rangle$ is either $|\uparrow\rangle$ or $|\downarrow\rangle$. With this we can now calculate the matrix elements of the Rabi Hamiltonian (3.11). Only the following are non-zero:

\[
\langle \downarrow n | \hat{H}_R | \downarrow n \rangle = \hbar n \omega_c, \quad (3.23)
\]
\[
\langle \uparrow n | \hat{H}_R | \uparrow n \rangle = \hbar (\omega_0 + n \omega_c), \quad (3.24)
\]
\[
\langle \uparrow n | \hat{H}_R | \downarrow n + 1 \rangle = \hbar g \sqrt{n + 1 T}, \quad (3.25)
\]
\[
\langle \uparrow n + 1 | \hat{H}_R | \uparrow n \rangle = \hbar g \sqrt{n + 1 T}, \quad (3.26)
\]
\[
\langle \downarrow n - 1 | \hat{H}_R | \downarrow n \rangle = \hbar g \sqrt{n T}. \quad (3.27)
\]
\[
\langle \downarrow n + 1 | \hat{H}_R | \uparrow n \rangle = \hbar g \sqrt{n + 1 T}. \quad (3.28)
\]

In the case of the Jaynes–Cummings Hamiltonian (3.21), the only non-zero elements are:

\[
\langle \downarrow n | \hat{H}_{JC} | \downarrow n \rangle = \hbar n \omega_c, \quad (3.29)
\]
\[
\langle \uparrow n | \hat{H}_{JC} | \uparrow n \rangle = \hbar (\omega_0 + n \omega_c), \quad (3.30)
\]
\[
\langle \uparrow n | \hat{H}_{JC} | \downarrow n + 1 \rangle = \hbar g \sqrt{n + 1 T}, \quad (3.31)
\]
\[
\langle \downarrow n + 1 | \hat{H}_{JC} | \uparrow n \rangle = \hbar g \sqrt{n + 1 T}. \quad (3.32)
\]
Explicit forms for the matrices are then (in the product basis \( \{ \uparrow n \} \)) written as

\[
H_R \cong h \begin{pmatrix}
0 & 0 & 0 & g & 0 & 0 & \cdots \\
0 & \omega_0 & g & 0 & 0 & 0 & \cdots \\
0 & g & \omega_k & 0 & 0 & g\sqrt{T} & \cdots \\
g & 0 & 0 & \omega_0 + \omega_k & g\sqrt{T} & 0 & \cdots \\
0 & 0 & 0 & g\sqrt{T} & 2\omega_k & 0 & \cdots \\
0 & g\sqrt{T} & 0 & 0 & \omega_0 + 2\omega_k & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\] (3.33)

and

\[
H_{JC} \cong h \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
0 & \omega_0 & g & 0 & 0 & 0 & \cdots \\
0 & g & \omega_k & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & \omega_0 + \omega_k & g\sqrt{T} & 0 & \cdots \\
0 & 0 & 0 & g\sqrt{T} & 2\omega_k & 0 & \cdots \\
0 & 0 & 0 & 0 & \omega_0 + 2\omega_k & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\] (3.34)

Here we use notation \( \cong \) to mean \( ' \)is represented by\( ' \), since the explicit matrix form of the operator depends on the basis [3]. From these it is clear that if the qubit and the cavity are decoupled \( (g = 0) \), the Hamiltonian matrices above are diagonal with eigenvalues

\[
E_{2n} = h n \omega_c, \quad n = 0, 1, 2, \ldots,
\]

\[
E_{2n+1} = h (\omega_0 + n \omega_c), \quad n = 0, 1, 2, \ldots,
\] (3.35, 3.36)

which means that the product basis \( \{ \uparrow n \} \) is the eigenbasis of the uncoupled Hamiltonian.

As mentioned above, no easy solution exists for the eigenproblem of the Rabi Hamiltonian. Jaynes–Cummings Hamiltonian, on the other hand, is block diagonal. The eigenvalues of a block-diagonal matrix can be calculated by solving the eigenvalues of individual block-matrices. The general block-matrix is

\[
H_{n,JC} \cong h \begin{pmatrix}
\omega_0 + n \omega_c & g\sqrt{n+1} \\
g\sqrt{n+1} & (n+1) \omega_c
\end{pmatrix} = h n \omega_c I + h \begin{pmatrix}
\omega_0 & g\sqrt{n+1} \\
g\sqrt{n+1} & \omega_c
\end{pmatrix}.
\] (3.37)

It is then enough to solve for the eigenvalues of the \( (2 \times 2) \) matrix in the latter form of Eq. (3.37). The eigenvalues of the Jaynes–Cummings Hamiltonian are therefore

\[
E_{gs} = 0,
\]

\[
E_{2n+1} = h n \omega_c + \frac{h}{2} (\omega_0 + \omega_k) - \frac{h}{2} \sqrt{\Delta^2 + 4 g^2 (n+1)}, \quad n = 0, 1, 2, \ldots,
\]

\[
E_{2n+2} = h n \omega_c + \frac{h}{2} (\omega_0 + \omega_k) + \frac{h}{2} \sqrt{\Delta^2 + 4 g^2 (n+1)}, \quad n = 0, 1, 2, \ldots,
\] (3.38, 3.39, 3.40)

where \( \Delta = |\omega_0 - \omega_k| \) is called the detuning parameter. Using these, we can calculate the corresponding eigenvectors. It is clear that for the ground state with energy \( E_{gs} = 0 \) the corresponding eigenvector is \( |0\rangle = (1, 0, 0, \ldots)^T = |\downarrow 0\rangle \). For the rest, we obtain after normalization

\[
|2n+1\rangle = \frac{1}{\sqrt{2 \Delta^2 - 2 \Delta \Omega}} \begin{pmatrix}
(\Delta - \Omega) |\uparrow n\rangle + 2 g \sqrt{n+1} |\downarrow n+1\rangle
\end{pmatrix}, \quad n = 0, 1, 2, \ldots,
\] (3.41)

\[
|2n+2\rangle = \frac{1}{\sqrt{2 \Delta^2 + 2 \Delta \Omega}} \begin{pmatrix}
(\Delta + \Omega) |\uparrow n\rangle + 2 g \sqrt{n+1} |\downarrow n+1\rangle
\end{pmatrix}, \quad n = 0, 1, 2, \ldots,
\] (3.42)

with the definition

\[
\Omega = \sqrt{\Delta^2 + 4 g^2 (n+1)}.
\] (3.43)

An important special case occurs when the qubit and the cavity are in resonance, \( \Delta = 0, \omega_0 = \omega_k \equiv \omega \), since then the exchange of energy between the qubit and the cavity is the most efficient. In this case, the energies are

\[
E_{2n+1} = h (n+1) \omega - h g \sqrt{n+1},
\]

\[
E_{2n+2} = h (n+1) \omega + h g \sqrt{n+1},
\] (3.44, 3.45)
and the state vectors can be written as

\[ |2n+1\rangle = \frac{1}{\sqrt{2}} (|\downarrow n+1\rangle - |\uparrow n\rangle), \quad (3.46) \]
\[ |2n+2\rangle = \frac{1}{\sqrt{2}} (|\downarrow n+1\rangle + |\uparrow n\rangle). \quad (3.47) \]

These are known as the Bell-states [11].

We are not able to produce such results for the Rabi Hamiltonian, but for completeness let us present the eigenvalues and eigenstates obtained from the second order time-independent perturbation theory [3, 30, 35], where we treat the interaction term (3.8) as the perturbation. In the non-degenerate case the energy eigenvalues are

\[ E_0 = -\frac{\hbar g^2}{\omega_0 + \omega_c}, \quad (3.48) \]
\[ E_{2n+1} = \hbar (\omega_0 + n\omega_c) + \frac{\hbar g^2(n+1)}{\omega_0 - \omega_c} + \frac{\hbar g^2n}{\omega_0 + \omega_c}, \quad n = 0, 1, 2, \ldots, \quad (3.49) \]
\[ E_{2n+2} = \hbar (n+1)\omega_c - \frac{\hbar g^2(n+1)}{\omega_0 - \omega_c} - \frac{\hbar g^2(n+2)}{\omega_0 + \omega_c}, \quad n = 0, 1, 2, \ldots, \quad (3.50) \]

with the (unnormalized) eigenstates

\[ |0\rangle = |\downarrow 0\rangle - \frac{g}{\omega_0 + \omega_c} |\uparrow 1\rangle, \quad (3.51) \]
\[ |2n+1\rangle = |\uparrow n\rangle + \frac{g\sqrt{n+1}}{\omega_0 - \omega_c} |\downarrow n+1\rangle + \frac{g\sqrt{n}}{\omega_0 + \omega_c} |\downarrow n-1\rangle, \quad n = 0, 1, 2, \ldots, \quad (3.52) \]
\[ |2n+2\rangle = |\downarrow n+1\rangle - \frac{g\sqrt{n+2}}{\omega_0 - \omega_c} |\uparrow n\rangle - \frac{g\sqrt{n+1}}{\omega_0 + \omega_c} |\uparrow n+2\rangle, \quad n = 0, 1, 2, \ldots. \quad (3.53) \]

We notice that the groundstate $|0\rangle$ is now affected by the coupling. If the qubit and the cavity are in resonance ($\omega_0 = \omega_c \equiv \omega$), one must use degenerate perturbation theory [3, 30, 35]. This does not change the ground state since it is always non-degenerate. For the excited states, one obtains for the energies (up to second order)

\[ E_{2n+1} = \hbar \omega(n+1) - \hbar g\sqrt{n+1} + \frac{\hbar g^2n}{2\omega}, \quad n = 0, 1, 2, \ldots, \quad (3.54) \]
\[ E_{2n+2} = \hbar \omega(n+1) + \hbar g\sqrt{n+1} - \frac{\hbar g^2(n+2)}{2\omega}, \quad n = 0, 1, 2, \ldots. \quad (3.55) \]

and for the (again unnormalized) eigenstates:

\[ |2n+1\rangle = \frac{1}{\sqrt{2}} (|\uparrow n\rangle + |\downarrow n+1\rangle) + \frac{g\sqrt{n}}{2\omega} |\downarrow n-1\rangle, \quad n = 0, 1, 2, \ldots, \quad (3.56) \]
\[ |2n+2\rangle = \frac{1}{\sqrt{2}} (|\uparrow n\rangle - |\downarrow n+1\rangle) - \frac{g\sqrt{n+2}}{2\omega} |\uparrow n+2\rangle, \quad n = 0, 1, 2, \ldots. \quad (3.57) \]

The corresponding results for the Jaynes–Cummings Hamiltonian can be obtained from Eqs. (3.48) - (3.57) by dropping out the last term from each equation. In the degenerate case, the second order perturbation theory gives exact results for the Jaynes–Cummings Hamiltonian.

Comparison of the exact numerically solved eigenvalues of the two Hamiltonians is shown in Figure 1, where the qubit and the cavity are in resonance. The eigenvalues start to differ notably at $g \approx 0.2\omega$. In Figure 2 the qubit has larger frequency than the cavity ($\omega_0 = 11\omega_c$). Here the Hamiltonians start to differ already at $g \approx 0.05\Delta$. 

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Figure 1: Six lowest eigenvalues of the Rabi (solid line) and Jaynes–Cummings (dashed line) Hamiltonians in resonance as a function of $g$. Parameters are: $\omega_c = 1$ and $\omega_0 = 1$.

Figure 2: Six lowest eigenvalues of the Rabi (solid line) and Jaynes–Cummings (dashed line) Hamiltonians with large detuning as a function of $g$. Parameters are: $\omega_c = 1$ and $\omega_0 = 11$. 
3.2. Environment

Let us then also define model for the environment and its coupling to the small system. One application of such model is the quantum mechanical treatment of damping and dissipation. Because of the energy conservation, one cannot add a term to the system Hamiltonian that would produce friction, i.e. loss of energy [2, 26, 27]. However, we can couple the small system to another system, thus allowing energy exchange between the two systems via the interaction term. The energy of the total two-component system is thus conserved, but from the point of view of the small system the energy is ‘lost’ into the environment, which is effectively seen as damping. The small system can also absorb energy from the environment, thus producing excitations in the small system [2, 26, 27].

A simple model for the environment is a reservoir consisting of infinite number of harmonic oscillators, i.e. bosons, which can be described by the Hamiltonian

\[ H_B = \hbar \sum_j \omega_j \hat{b}_j^\dagger \hat{b}_j. \]  

(3.58)

Here \( \omega_j \), \( \hat{b}_j \) and \( \hat{b}_j^\dagger \) are the angular frequency, creation and annihilation operator of the \( j^{th} \) oscillator, respectively. The coupling between the system and the environment is assumed to be bilinear. It can be described by the interaction Hamiltonian

\[ H_{SB} = \hbar q \xi, \]  

(3.59)

where \( q \) is a Hermitian operator of the system. The Hermitian operator \( \xi \) of the reservoir can be written as

\[ \xi = \sum_j g_j (\hat{b}_j^\dagger + \hat{b}_j), \]  

(3.60)

where \( g_j \) is a coefficient describing the strength of the interaction between the small system and the \( j^{th} \) oscillator of the environment. This model is widely used in the literature [1, 2, 5, 6, 8, 11, 12, 13, 14, 15, 19, 25, 26, 27, 41, 42]. In the qubit-cavity system, we assume that only the cavity is coupled to the environment, so we can write \( q \) as

\[ q = q_0 (\hat{a}^\dagger + \hat{a}), \]  

(3.61)

where \( q_0 \) is the characteristic length scale which determines the magnitude of the zero-point fluctuations in the cavity. The total Hamiltonian of the qubit-cavity system coupled to the bosonic reservoir can then be written as

\[ H_{tot} = H_R + H_B + H_{SB}, \]  

(3.62)

\[ = \hbar \omega_c \hat{a}^\dagger \hat{a} + \hbar \omega_b \sigma_z \sigma_z + h g (\hat{a}^\dagger + \hat{a}) (\sigma_+ + \sigma_-) + \hbar \sum_j \omega_j \hat{b}_j^\dagger \hat{b}_j + \hbar q_0 (\hat{a}^\dagger + \hat{a}) \sum_j g_j (\hat{b}_j^\dagger + \hat{b}_j). \]  

(3.63)

Correlation function \( \langle \xi(t) \xi(t') \rangle \) (written in the interaction picture) characterizes the force that the reservoir exerts to the small system. We denote it by \( L(t - t') \):

\[ L(t - t') \equiv \langle \xi(t) \xi(t') \rangle. \]  

(3.64)

This quantity determines the dynamics of the small system. For example, if the environmental coupling is weak, the transition rates between the system eigenstates \( |m \rangle \) and \( |n \rangle \) with energies \( \hbar \omega_m \) and \( \hbar \omega_n \), respectively, can be approximated by the Fermi’s golden rule, which we write in the form [10, 11, 12, 13]

\[ \Gamma_{m \rightarrow n} = | \langle n | \hat{q} | m \rangle |^2 L(-\omega_{mn}), \]  

(3.65)

where \( \omega_{mn} \equiv \omega_n - \omega_m \) and \( L \) is the spectrum of the environmental fluctuations, obtained from the correlation function by the Fourier transform

\[ \tilde{L}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} L(t). \]  

(3.66)

The correlation function can be recovered from the spectrum of the environmental fluctuations by the inverse Fourier transform:

\[ L(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{L}(\omega). \]  

(3.67)

For future purposes we calculate some analytical results for the environmental correlation function. In the interaction picture, we have that \( \hat{b}_{j,1}(t) = \hat{b}_{j}(e^{-i\omega_j t}), \) and, thus,

\[ \langle \left[ \hat{b}_{j,1}(t) + \hat{b}_{j,1}^\dagger(t) \right] \left[ \hat{b}_{j,1}^\dagger(t) + \hat{b}_{j,1}(t') \right] \rangle = N_j e^{i\omega_j (t-t')} + (1 + N_j) e^{-i\omega_j (t-t')}. \]  

(3.68)
The expectation values of operators $\hat{b}_j^\dagger \hat{b}_j$ and $\hat{b}_j \hat{b}_j$ vanish since we assume that the oscillators are in the thermal equilibrium, i.e. the number of quanta is conserved [2]. This justifies the lower index $B$, standing for Bath in Eq. (3.58). Thus, we can write the average number of quanta as [1, 2, 11, 12, 43]:

$$N_j = \langle \hat{b}_j^\dagger \hat{b}_j \rangle = \frac{1}{e^{\beta \omega_j} - 1}, \quad \beta = \frac{1}{k_B T}, \quad (3.69)$$

where $k_B$ is the Boltzmann constant and $T$ is the temperature of the environment. By assuming that the oscillators are independent, we obtain the environmental correlation function [2, 5, 6, 8, 13, 44]

$$L(t - t') = \left\langle \tilde{\xi}_j(t) \tilde{\xi}_i(t') \right\rangle = \sum_j c_j^2 \left[ N_j e^{i \omega_j (t - t')} + (1 + N_j) e^{-i \omega_j (t - t')} \right] \quad (3.70)$$

$$= \frac{\hbar}{\pi} \int_0^\infty d\omega J(\omega) \left\{ N(\omega) e^{i \omega (t - t')} + [1 + N(\omega)] e^{-i \omega (t - t')} \right\} \quad (3.71)$$

where last equality holds for odd spectral densities $J(-\omega) = -J(\omega)$. Here we have also used the definitions of the Dirac delta function

$$\delta(\omega - \Omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i(\omega - \Omega) t} \quad (3.72)$$

and the Heaviside step function

$$\Theta(\omega) = \begin{cases} 1, & \omega > 0 \\ 0, & \omega < 0 \end{cases} \quad (3.73)$$

We notice that the spectral density $J(\omega)$ determines the system dynamics [5, 6]. Usually one approximates $J(\omega)$ with a continuous function. One possibility is to use ohmic spectral density $J(\omega) = \eta \omega$, which leads to Johnson–Nyquist relation [2]:

$$\tilde{L}(\omega) = \frac{2h \eta \omega}{1 - e^{-\beta \omega}} \quad (3.74)$$

However, this leads to a divergent spectrum [5, 10]. More physical model can be obtained by using Drude model

$$J(\omega) = \frac{\eta \omega}{(1 + \omega^2/\omega_D^2)^n}, \quad n = 1, 2, \ldots \quad (3.80)$$

where $\omega_D$ is so-called Drude cutoff frequency. Its inverse defines the characteristic correlation time for the environment [5, 6, 8, 10]. If $\omega \ll \omega_D$, this approaches the ohmic spectral density. Here $\eta$ is a coefficient which governs the damping of the system. On the other hand, $\tilde{L}(\omega)$ in Eq. (3.77) describes the fluctuations, or random noise, which the environment causes to the system. Thus, Eq. (3.77) tells us that the fluctuation and dissipation are related. This is known as the fluctuation-dissipation theorem [1, 2, 26]. In classical mechanics damping could be included by adding a friction term to the equations of motion. In quantum mechanics our attempt to include damping has indeed produced dissipation, but simultaneously we have also obtained fluctuations, absorption of the energy from the environment to the system.

The integral in Eq. (3.72) can be solved at least for the Drude model (3.81) by treating the real and imaginary parts separately and using the Cauchy residue theorem. The imaginary part $L_1(t)$ is relatively simple. The real
part $L_R(t)$, on the other hand, is difficult, but it can be determined with $L(t)$ and $L_4(t)$. We use $n = 2$ in the Drude model and obtain for the imaginary part $L_4(t)$

$$
L_4(t-t') = -\frac{\hbar}{\pi} \int_0^\infty d\omega J(\omega) \sin[\omega(t-t')], \quad (3.82)
$$

$$
= -\frac{\hbar}{2\pi} \int_{-\infty}^\infty d\omega J(\omega) \sin[\omega(t-t')], \quad (3.83)
$$

$$
= -\frac{\hbar}{2\pi} \int_{-\infty}^\infty d\omega \frac{\eta \omega}{(1 + \omega^2/\omega_D^2)\omega} \sin[\omega(t-t')], \quad (3.84)
$$

$$
= -\frac{\eta \omega_D^2 \hbar}{2\pi} \int_{-\infty}^\infty d\omega \frac{\omega \sin[\omega(t-t')]}{(\omega^2 + \omega_D^2)^2}, \quad (3.85)
$$

$$
= -\frac{\eta \omega_D^2 \hbar}{2\pi} \text{Im} \int_{-\infty}^\infty d\omega \frac{\omega e^{i\omega(t-t')}}{(\omega^2 + \omega_D^2)^2(\omega - i\omega_D)^2}. \quad (3.86)
$$

$$
= -\frac{\eta \omega_D^2 \hbar}{2\pi} \text{Im} \int_{-\infty}^\infty d\omega \frac{\omega e^{i\omega(t-t')}}{(\omega + i\omega_D)^2(\omega - i\omega_D)^2}. \quad (3.87)
$$

The integrand has second order poles at $\omega = \pm i\omega_D$. We extend the integration to complex plane and choose the integration contour to be such that only $\omega = i\omega_D$ is located inside the curve. By using the residue theorem, we obtain

$$
\int_{-\infty}^\infty d\omega \frac{\omega e^{i\omega(t-t')}}{(\omega + i\omega_D)^2(\omega - i\omega_D)^2} = 2\pi i \text{Res} \left[ \frac{\omega e^{i\omega(t-t')}}{(\omega + i\omega_D)^2(\omega - i\omega_D)^2} \right], \quad (3.88)
$$

Calculating the residue results in

$$
\text{Res} \left[ \frac{\omega e^{i\omega(t-t')}}{(\omega + i\omega_D)^2(\omega - i\omega_D)^2} \right] = \frac{\text{sgn}(t-t')|t-t'|e^{-\omega_D|t-t'|}}{4\omega_D}. \quad (3.89)
$$

Therefore we obtain

$$
L_4(t-t') = -\frac{\eta \omega_D^2 \hbar}{4} \text{sgn}(t-t')|t-t'|e^{-\omega_D|t-t'|}. \quad (3.90)
$$

For future purposes we also need an expression for the real part of $\tilde{L}(\omega)$. We write $\tilde{L}(\omega) = L_R(\omega) + i\tilde{L}_I(\omega)$, which implies that

$$
\tilde{L}_R(\omega) = \tilde{L}(\omega) - i\tilde{L}_I(\omega). \quad (3.91)
$$

Thus, we have to calculate $\tilde{L}_I(\omega)$. Proceeding similarly as in Eqs. (3.74) - (3.77), we obtain

$$
\tilde{L}_I(\omega) = \int_{-\infty}^\infty dt e^{i\omega t} \tilde{L}_4(t) = \frac{\hbar}{\pi} \int_{-\infty}^\infty d\Omega e^{i\omega \Omega} J(\Omega) \sin(\Omega t) \quad (3.92)
$$

$$
= -\frac{\hbar}{2\pi} \int_{-\infty}^\infty d\Omega J(\Omega) \int_{-\infty}^\infty d\omega e^{i\omega t} \left[ e^{i\Omega t} - e^{-i\Omega t} \right] \quad (3.93)
$$

$$
= -\frac{2\pi \hbar}{2\pi} \int_{-\infty}^\infty d\Omega J(\Omega) \left[ \delta(\Omega + \omega) - \delta(-\Omega + \omega) \right] \quad (3.94)
$$

$$
= -i\hbar J(\omega) \Theta(\omega) - J(-\omega) \Theta(-\omega). \quad (3.95)
$$

We now obtain an expression for $\tilde{L}_R(\omega)$ by using Eqs. (3.76) and (3.95)

$$
\tilde{L}_R(\omega) = \tilde{L}(\omega) - i\tilde{L}_I(\omega) = \hbar \left[ 1 + 2N(\omega) \right] [J(\omega) \Theta(\omega) - J(-\omega) \Theta(-\omega)], \quad (3.96)
$$

$$
= \hbar \coth(\beta \hbar \omega/2) [J(\omega) \Theta(\omega) - J(-\omega) \Theta(-\omega)], \quad (3.97)
$$

$$
= \hbar \coth(\beta \hbar \omega/2) J(\omega), \quad (3.98)
$$

where in the first line we have used the fact that $N(\omega) + 1 = -N(-\omega)$. The last equality holds if $J(\omega)$ is odd [13], which is the case for the Drude model. [10]
4. Time evolution

Now that we have defined our small quantum system and the environment, let us discuss how the state of the small system evolves in time. Thus, we need a dynamical equation for the reduced density operator $\hat{\rho}_S(t)$. Here we present two different methods for obtaining $\hat{\rho}_S(t)$: Lindblad master equations with the Born–Markov approximations and a formally exact stochastic Liouville–von Neumann (SLN) equation. We first derive the master equations that are widely used in the literature [1, 2, 4, 8, 11, 12, 13, 14, 15, 19, 20, 24, 28, 40, 42, 43, 45, 46] and then discuss their properties and validities. After that we consider the stochastic Liouville–von Neumann equation [5, 6, 8, 9, 10, 42, 44, 47, 48, 49].

4.1. Master equations

4.1.1. Derivation

We start the derivation of the master equation by considering the von Neumann equation in the interaction picture (2.40) for the whole system (i.e. including the bath) density operator:

$$i\hbar \frac{d\hat{\rho}_I(t)}{dt} = [\hat{H}_I(t), \hat{\rho}_I(t)], \quad (4.1)$$

which can also be written in the integral form

$$\hat{\rho}_I(t) = \hat{\rho}_I(t_0) - i\frac{\hbar}{\hbar} \int_{t_0}^t ds \left[ \hat{H}_I(s), \hat{\rho}_I(s) \right], \quad (4.2)$$

For the future purposes, we set the initial time $t_0 = 0$ without any loss of generality. We insert Eq. (4.2) into the right-hand side of Eq. (4.1) and take the trace over the bath. The resulting equation can be written as [2, 25, 26, 27, 50]

$$\frac{d\hat{\rho}_{S,1}(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t ds \text{Tr}_B \left[ \hat{H}_I(t), \left[ \hat{H}_I(s), \hat{\rho}_I(s) \right] \right], \quad (4.3)$$

where we assume that

$$\text{Tr}_B[\hat{H}_I(t), \hat{\rho}_I(0)] = 0. \quad (4.4)$$

Equation (4.3) is not yet the equation we are looking for, since it still contains the density matrix of the total system. To eliminate $\hat{\rho}_I(t)$, we perform the Born approximation by assuming that the coupling between the reservoir and the small system is weak, i.e. the small system has only small influence on the reservoir. Because of this, the density operator of the whole system can be approximated to be a Kroenecker product of the density operators of the small system and the reservoir: [1, 2, 4, 25, 26, 27, 50]

$$\hat{\rho}_I(t) \approx \hat{\rho}_{S,1}(t) \otimes \hat{\rho}_{B,1}. \quad (4.5)$$

Inserting this into Eq. (4.3) we then obtain an equation for the density operator of the small system

$$\frac{d\hat{\rho}_{S,1}(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t ds \text{Tr}_B \left[ \hat{H}_I(t), \left[ \hat{H}_I(s), \hat{\rho}_{S,1}(s) \otimes \hat{\rho}_{B,1} \right] \right]. \quad (4.6)$$

To simplify this even further we make the Markov approximation, where in the integrand we replace $\hat{\rho}_{S,1}(s)$ with $\hat{\rho}_{S,1}(t)$ and obtain the Redfield equation [1]:

$$\frac{d\hat{\rho}_{S,1}(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t ds \text{Tr}_B \left[ \hat{H}_I(t), \left[ \hat{H}_I(s), \hat{\rho}_{S,1}(t) \otimes \hat{\rho}_{B,1} \right] \right]. \quad (4.7)$$

Substituting here the interaction Hamiltonian $\hat{H}_I(t) = \hbar \hat{q}_I(t) \hat{\xi}_I(t)$, we obtain

$$\frac{d\hat{\rho}_{S,1}(t)}{dt} = -\int_0^t ds \text{Tr}_B \left[ \hat{q}_I(t) \hat{\xi}_I(t), \left[ \hat{q}_I(s) \hat{\xi}_I(s), \hat{\rho}_{S,1}(t) \otimes \hat{\rho}_{B,1} \right] \right]. \quad (4.8)$$

If we assume that the reservoir forgets all changes induced to it by the small system much faster than the small system can change its state, i.e. we assume short correlation time for the environment compared to the time scales of the small system [1, 2, 13, 25, 26, 27]. We can therefore conclude the Markov approximation by letting $t \to \infty$.
We can write the terms containing the trace over the reservoir degrees of freedom as

\[ \Tr_B \left[ \hat{g}_1(t) \hat{g}_1(s) \rho_{B,1} \right] \]

by the inverse Fourier transform of the spectral density as \[13\]

\[
\rho_{S,1}(t) \hat{q}_1(t) - \hat{q}_1(t) \rho_{S,1}(t) \hat{q}_1(t) \]

\[ \Tr_B \left[ \hat{g}_1(t) \hat{g}_1(s) \rho_{B,1} \right] \].

We can write the terms containing the trace over the reservoir degrees of freedom as

\[
\Tr_B \left[ \hat{g}_1(t) \hat{g}_1(s) \rho_{B,1} \right] = \left\langle \hat{g}_1(t) \hat{g}_1(s) \right\rangle ,
\]

which is the correlation function \( L(t - s) \) we discussed in Section 3. Because the reservoir is in thermal equilibrium, we make a change of variables by substituting \( \tau = t - s \) and obtain

\[
\left\langle \hat{g}_1(t) \hat{g}_1(s) \right\rangle = \left\langle \hat{g}_1(\tau) \hat{g}_1(0) \right\rangle = L(\tau),
\]

(4.11)

\[
\left\langle \hat{g}_1(s) \hat{g}_1(t) \right\rangle = \left\langle \hat{g}_1(-\tau) \hat{g}_1(0) \right\rangle = L(-\tau).
\]

(4.12)

In Eq. (3.66), we defined the spectral density \( \tilde{E} \) of the reservoir as the Fourier transform of the correlation function \( L(t) \), and in Eqs. (3.76) and (3.77) solved it analytically. We can therefore replace the correlation functions by the inverse Fourier transform of the spectral density as \[13\]

\[
L(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega \tau} L(\omega),
\]

(4.13)

\[
L(-\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega \tau} \tilde{L}(\omega).
\]

(4.14)

As a consequence, we can write the master equation (4.9) as

\[
\frac{d\rho_{S,1}(t)}{dt} = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{0}^{\infty} d\tau e^{-i\omega \tau} \left\{ \hat{L}(\omega) \left[ \dot{\hat{q}}_1(t) \hat{q}_1(t - \tau) \hat{\rho}_{S,1}(t) - \hat{q}_1(t - \tau) \hat{\rho}_{S,1}(t) \dot{\hat{q}}_1(t) \right] + \right. \]

\[
\left. \hat{L}(-\omega) \left[ \hat{\rho}_{S,1}(t) \dot{\hat{q}}_1(t - \tau) \hat{q}_1(t) - \dot{\hat{q}}_1(t) \hat{\rho}_{S,1}(t) \hat{q}_1(t - \tau) \right] \right\} .
\]

(4.15)

Above, we have product terms of the form \( \dot{\hat{q}}_1(t - \tau) \hat{q}_1(t) \), in which the time-evolution operator \( \hat{U}_0(t, 0) \) operates on \( \hat{q} \). Therefore, it is convenient to write the operator \( \hat{q} \) in the eigenbasis of the time-evolution operator. We therefore have to solve the eigenvalue problem

\[
\hat{U}_0(t, 0) | n \rangle = u_n(t, 0) | n \rangle \]

(4.16)

Using the equation (2.29) with \( \hat{H}_0 = \hat{H}_S + \hat{H}_B \), we obtain \[13\]

\[
\frac{d\hat{U}_0(t, 0)}{dt} | n \rangle = i\hbar \frac{d}{dt} u_n(t, 0) | n \rangle = \hat{H}_S \hat{U}_0(t, 0) | n \rangle = u_n(t, 0) \hat{H}_S | n \rangle ,
\]

(4.17)

where we have assumed that \( | n \rangle \) are time-independent. One can see that the states \( | n \rangle \) are also the eigenstates of the system Hamiltonian

\[
\hat{H}_S | n \rangle = i\hbar \frac{d}{dt} u_n(t, 0) | n \rangle = \hbar \omega_n | n \rangle ,
\]

(4.18)

from which we can solve

\[
u_n(t, 0) = e^{-i\omega_n t}.
\]

(4.19)

Therefore, the operator \( \hat{q}_1(t) \) can be written as

\[
\hat{q}_1(t) = \sum_{nm} \hat{q}_{nm} e^{-i\omega_n t},
\]

(4.20)

where \( \omega_{nm} \equiv \omega_n - \omega_m \) and \( \hat{q}_{nm} = \langle n | \hat{q} | m \rangle \), \( \hat{x}_{nm} \) with \( \hat{x}_{nm} = | n \rangle \langle m | \). Thus, in the master equation (4.15) we have terms of the form

\[
\hat{q}_1(t) \hat{q}_1(t - \tau) = \sum_{nm} \hat{q}_{nm} \hat{q}_{nm} e^{-i(\omega_m t + \omega_n t)} e^{i\omega_m t}.
\]

(4.21)

In order to remove \( t \)-dependence, we choose only terms for which \( k = m \) and \( l = n \) and obtain

\[
\hat{q}_1(t) \hat{q}_1(t - \tau) \approx \sum_{mn} \hat{q}_{mn} \hat{q}_{nm} e^{i\omega_m t} = \sum_{n \rightarrow n} \left( \hat{q}_{nm} \hat{q}_{nm} e^{i\omega_m t} + \hat{q}_{nm} \hat{q}_{nm} e^{i\omega_m t} + \sum_{n} \hat{q}_{nm} \hat{q}_{nm} \right).
\]

(4.22)
This procedure is called the secular approximation [11, 12, 13, 20]. The terms in the master equation (4.15) are thus approximated by [13]

\[ \dot{q}_n(t) \approx \sum_{n<m} \left( \dot{q}_{nm} \dot{q}_{nm} \right) e^{-i\omega_{nm} \tau} + \dot{q}_m \dot{q}_{nm} e^{i\omega_{nm} \tau} \]

\[ \dot{q}_m(t) = \sum_{m<n} \left( \dot{q}_{nm} \dot{q}_{nm} \right) e^{-i\omega_{nm} \tau} + \dot{q}_m \dot{q}_{nm} e^{i\omega_{nm} \tau} \]

With these we can write the master equation (4.15) as

\[
\frac{d\hat{\rho}_{S}(t)}{dt} = -\sum_{\omega_{nm} > 0} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \times \left[ \left[ L(\omega) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} \right] + L(-\omega) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) + \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} \right] \right] \int_{0}^{\infty} d\tau e^{-i(\omega + \omega_{nm}) \tau} \\
+ \left[ L(\omega) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} \right] + L(-\omega) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) + \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} \right] \int_{0}^{\infty} d\tau e^{-i(\omega - \omega_{nm}) \tau} \\
- \sum_{n} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left[ L(\omega) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} \right] + L(-\omega) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) + \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} \right] \int_{0}^{\infty} d\tau e^{-i\omega \tau}.
\]

The integrals can also be written as [13]

\[
\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{0}^{\infty} d\tau e^{-i(\omega' - \omega) \tau} L(\omega) = \int_{0}^{\infty} d\tau \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i(\omega' - \omega) \tau} L(\omega),
\]

\[
= \int_{0}^{\infty} d\tau e^{i\omega' \tau} L(\tau),
\]

\[
= \frac{1}{2} L(\omega') + i \text{Im} \left( \int_{0}^{\infty} d\tau e^{i\omega' \tau} L(\tau) \right),
\]

where symmetry relation \( L' (\tau) = L(-\tau) \) was used in the last equality. The imaginary part is usually neglected in Lindblad master equations since it causes a Lamb shift of the energy levels [1, 2, 13], which is usually only a small correction. Replacing this calculation for the rest of the terms results in

\[
\frac{d\hat{\rho}_{S}(t)}{dt} = \frac{1}{2} \sum_{\omega_{nm} > 0} \left[ L(-\omega_{nm}) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} + \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} \right] \\
+ L(\omega_{nm}) \left[ \dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) + \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} \right] \\
+ \frac{1}{2} \sum_{n} L(0) \left[ 2\dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} - \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} \right].
\]

By combining equal terms, we obtain

\[
\frac{d\hat{\rho}_{S}(t)}{dt} = \frac{1}{2} \sum_{\omega_{nm} > 0} \left[ L(-\omega_{nm}) \left[ 2\dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} + \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} \right] \\
+ \frac{1}{2} \sum_{\omega_{nm} > 0} L(\omega_{nm}) \left[ 2\dot{q}_{nm} \dot{q}_{nm} \right] \hat{\rho}_{S}(t) - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} + \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} \right] \\
+ \frac{1}{2} \sum_{n} L(0) \left[ 2\dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} - \dot{q}_{nm} \hat{\rho}_{S}(t) \dot{q}_{nm} - \hat{\rho}_{S}(t) \dot{q}_{nm} \dot{q}_{nm} \right].
\]

The transition rates between states \( |n \rangle \) and \( |m \rangle \) were already defined in Eq. (3.65) as

\[
\Gamma_{m \rightarrow n} = |\langle n | \dot{q} | m \rangle|^2 L(-\omega_{nm}).
\]
Thus, we can write Eq. (4.32) as [11, 13]

\[
\frac{d\hat{S}_{1}(t)}{dt} = \frac{1}{2} \sum_{\alpha_{nm} > 0} \Gamma_{n-m} \left[ 2\hat{n}_{nm}\hat{S}_{1}(t)\hat{n}_{nm} - \hat{n}_{nm}\hat{n}_{nm}\hat{S}_{1}(t) - \hat{S}_{1}(t)\hat{n}_{nm}\hat{n}_{nm} \right] \\
+ \frac{1}{2} \sum_{\alpha_{nm} > 0} \Gamma_{m-n} \left[ 2\hat{n}_{nm}\hat{S}_{1}(t)\hat{n}_{nm} - \hat{n}_{nm}\hat{n}_{nm}\hat{S}_{1}(t) - \hat{S}_{1}(t)\hat{n}_{nm}\hat{n}_{nm} \right] \\
+ \frac{1}{2} \sum_{\alpha_{nm}} \Gamma_{n-m} \left[ 2\hat{n}_{nm}\hat{S}_{1}(t)\hat{n}_{nm} - \hat{n}_{nm}\hat{n}_{nm}\hat{S}_{1}(t) - \hat{S}_{1}(t)\hat{n}_{nm}\hat{n}_{nm} \right].
\]

(4.34)

The first row in Eq. (4.34) describes absorption from the reservoir and the second row emission to the reservoir. The third row describes possible dephasing processes in the system. Note that in this master equation the transitions are between the eigenstates \( |n \rangle \) of the system Hamiltonian \( \hat{H}_S \) [11, 12, 13].

However, in the literature this master equation is seldom used. Instead, one often uses the so called quantum optical master equation. Let us derive that next. We begin by considering the qubit-cavity system described in Section 3 and assume that there is no coupling between the qubit and the cavity, i.e. \( g = 0 \) in Eq. (3.11). Thus, Eq. (4.20) becomes

\[
\hat{q}_1(t) = q_0 \left( \hat{a}_1(t) + \hat{a}_1^{\dagger}(t) \right) \approx q_0 \left( \hat{a}e^{-i\omega t} + \hat{a}^{\dagger}e^{i\omega t} \right).
\]

(4.35)

In this case Eqs. (4.23) - (4.26) are thus reduced to

\[
\hat{q}_1(t)\hat{q}_1(t-t')\hat{\rho}_{S,1}(t) \approx q_0^2 \left( \hat{a}\hat{a}e^{-i\omega t} + \hat{a}^{\dagger}\hat{a}e^{i\omega t} \right) \hat{\rho}_{S,1}(t),
\]

(4.36)

\[
\hat{q}_1(t-t')\hat{\rho}_{S,1}(t)\hat{q}_1(t) \approx q_0^2 \hat{\rho}_{S,1}(t)\hat{a}e^{i\omega t} + q_0^2 \hat{\rho}_{S,1}(t)\hat{a}e^{-i\omega t},
\]

(4.37)

\[
\hat{\rho}_{S,1}(t)\hat{q}_1(t-t')\hat{q}_1(t) \approx q_0^2 \hat{\rho}_{S,1}(t)\left( \hat{a}\hat{a}e^{i\omega t} + \hat{a}^{\dagger}\hat{a}e^{-i\omega t} \right),
\]

(4.38)

\[
\hat{q}_1(t)\hat{\rho}_{S,1}(t)\hat{q}_1(t-t') \approx q_0^2 \hat{\rho}_{S,1}(t)\hat{a}e^{-i\omega t} + q_0^2 \hat{\rho}_{S,1}(t)\hat{a}e^{i\omega t},
\]

(4.39)

where instead of the secular approximation we performed the rotating wave approximation with respect to timescales \( t > 1/\alpha_c \). The master equation is then reduced to

\[
\frac{d\hat{\rho}_{S,1}(t)}{dt} = \frac{1}{2}\hat{q}_0^2L(-\alpha_c) \left[ 2\hat{a}\hat{\rho}_{S,1}(t)\hat{a} - \hat{a}\hat{a}\hat{\rho}_{S,1}(t) - \hat{\rho}_{S,1}(t)\hat{a}\hat{a} \right] \\
+ \frac{1}{2}\hat{q}_0^2L(\alpha_c) \left[ 2\hat{a}\hat{\rho}_{S,1}(t)\hat{a} - \hat{a}\hat{a}\hat{\rho}_{S,1}(t) - \hat{\rho}_{S,1}(t)\hat{a}\hat{a} \right].
\]

(4.40)

Using Eq. (3.76), we can write this as

\[
\frac{d\hat{\rho}_{S,1}(t)}{dt} = \frac{\kappa(\alpha_c)}{2} \left[ N(\alpha_c) + 1 \right] \left[ 2\hat{a}\hat{\rho}_{S,1}(t)\hat{a} - \hat{a}\hat{a}\hat{\rho}_{S,1}(t) - \hat{\rho}_{S,1}(t)\hat{a}\hat{a} \right] \\
+ \frac{\kappa(\alpha_c)}{2} \left[ N(\alpha_c) - 1 \right] \left[ 2\hat{a}\hat{\rho}_{S,1}(t)\hat{a} - \hat{a}\hat{a}\hat{\rho}_{S,1}(t) - \hat{\rho}_{S,1}(t)\hat{a}\hat{a} \right],
\]

(4.41)

where we have defined [2, 13]

\[
\kappa(\alpha) = 2\hbar\tilde{\alpha}^2J(\alpha) = \frac{2\hbar\tilde{\alpha}^2\eta\alpha}{(1 + \alpha^2/\alpha_c^2)^2},
\]

(4.42)

and \( N(\alpha) \) is the average number of quanta in the reservoir with the angular frequency \( \omega \) at temperature \( T \), as defined in Eq. (3.69):

\[
N(\alpha) = \frac{1}{e^{\alpha T} - 1}.
\]

(4.43)

Interaction between the qubit and the cavity can be added to the Eq. (4.41) by simply adding the term \(-\frac{i}{\hbar} [\hat{H}_I, \hat{\rho}_{S,1}(t)]\) [2]. After this we change from the interaction picture back to the Schrödinger picture, which transforms Eq. (4.41) into

\[
\frac{d\hat{\rho}_S(t)}{dt} = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S(t)] + \frac{\kappa(\alpha_c)}{2} \left[ N(\alpha_c) + 1 \right] \left[ 2\hat{a}\hat{\rho}_S(t)\hat{a} - \hat{a}\hat{a}\hat{\rho}_S(t) - \hat{\rho}_S(t)\hat{a}\hat{a} \right] \\
+ \frac{\kappa(\alpha_c)}{2} \left[ N(\alpha_c) - 1 \right] \left[ 2\hat{a}\hat{\rho}_S(t)\hat{a} - \hat{a}\hat{a}\hat{\rho}_S(t) - \hat{\rho}_S(t)\hat{a}\hat{a} \right],
\]

(4.44)

which is throughout the rest of the thesis referred to as the quantum optical (QO) master equation. This equation is widely used in the literature, especially in quantum optics [1, 2, 4, 11, 12, 14, 15, 24, 25, 26, 27, 28, 40, 42, 45].
where the coupling $g$ can be treated as a small correction to the uncoupled system. Here the Hamiltonian operator $\hat{H}_S$ is either the Rabi Hamiltonian (3.11) or the Jaynes–Cummings Hamiltonian (3.21).

Using the same notation for the transition rates and changing to the Schrödinger picture, Eq. (4.34) is transformed into

$$
\frac{d\hat{\rho}_S(t)}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_S, \hat{\rho}_S(t) \right] + \frac{1}{2} \sum_{\omega_{hm} > 0} \kappa(\omega_{hm}) \left[ |n\rangle \langle n| \hat{q} |m\rangle \langle m| - |m\rangle \langle m| \hat{q}^\dagger |n\rangle \langle n| + |n\rangle \langle n| \hat{q}^\dagger |m\rangle \langle m| - |m\rangle \langle m| \hat{q} |n\rangle \langle n| \right] \left[ 2\hat{\pi}_{nm}\hat{\rho}_S(t) - \hat{\pi}_{nm}\hat{\rho}_S(t) - \hat{\rho}_S(t)\hat{\pi}_{nm}^\dagger \right] \hat{\pi}_{nm}^\dagger,
$$

where we have neglected the dephasing terms since they vanish in the case of bilinear coupling between the harmonic oscillator and bosonic bath. From now on, this master equation is referred to as the eigenstate (ES) master equation, since the transitions caused by the operators $\hat{\pi}_{nm}$ occur between the eigenstates of the small system Hamiltonian. The transitions in the quantum optical master equation occur between the eigenstates of the cavity, instead. \[1, 4, 8, 11, 12, 13, 14, 15, 19, 20, 43, 46\]

This concludes our derivation of the master equations, which are of the Lindblad form. Let us gather here all the assumptions that we made during the derivation. We assumed that the coupling between the small system and the bath is weak (i.e. $\kappa$ coefficients are small compared to the transition energies in the system). We also assumed short memory for the bath: all changes in the environment caused by the system disappear much faster than the system can change its state. This allowed us to expand the time integration in Eq. (4.27) to the infinity. This is known as the Markov approximation. We also made the secular approximation by discarding rapidly oscillating terms in Eqs. (4.23) - (4.26). In the case of the quantum optical master equation we also neglected the coupling between the cavity and the qubit while formulating the dissipators, and instead of the secular approximation for the transition angular frequencies $\omega_{hm}$ we performed the rotating wave approximation with respect to the cavity angular frequency $\omega_c$. Finally, we neglected the Lamb shift of the energy levels caused by the environment.

Because of these assumptions, the quantum optical master equation should be valid if $g, \kappa(\omega_c) \ll \Delta_c$. The eigenstate master equation, on the other hand, should be valid for all $g$, but only if $\kappa_{max} \ll g$. This is because in the quantum optical master equation the rotating wave approximation was done for angular frequencies of the order of $\omega_c$, while in the eigenstate master equation the secular approximation was done for angular frequencies $\omega_{hm}$, some of which are of the order of $g$. \[11, 12\]

### 4.1.2. Component forms of the master equations

Let us here write the quantum optical master equation for the individual components of the density matrix written in the product space basis \{$|\downarrow n\rangle$\}. We start by using the Rabi Hamiltonian (3.11) and obtain

$$
\frac{d\rho_{\downarrow m\uparrow n}}{dt} = \kappa(\omega_c)\left[ N(\omega_c) + 1 \right] \left[ \sqrt{(m+1)(n+1)} \rho_{\downarrow m+1\uparrow n+1} - \frac{1}{2}(m+n)\rho_{\downarrow m\uparrow n} \right] + \kappa(\omega_c)\left[ N(\omega_c) \right] \left[ \sqrt{mn} \rho_{\downarrow m\uparrow n} - \frac{1}{2}(m+n+2)\rho_{\downarrow m\uparrow n} \right] + \frac{i}{2} \left[ \omega_c(n-m)\rho_{\downarrow m\uparrow n} + g \left( \sqrt{n+1}\rho_{\downarrow m+1\uparrow n} - \sqrt{m+1}\rho_{\downarrow m\uparrow n+1} \right) \right] + g \left( \sqrt{n+1}\rho_{\downarrow m+1\uparrow n} - \sqrt{m+1}\rho_{\downarrow m\uparrow n+1} \right),
$$

$$
\frac{d\rho_{\downarrow m\downarrow n}}{dt} = \kappa(\omega_c)\left[ N(\omega_c) + 1 \right] \left[ \sqrt{(m+1)(n+1)} \rho_{\downarrow m+1\downarrow n+1} - \frac{1}{2}(m+n)\rho_{\downarrow m\downarrow n} \right] + \kappa(\omega_c)\left[ N(\omega_c) \right] \left[ \sqrt{mn} \rho_{\downarrow m\downarrow n} - \frac{1}{2}(m+n+2)\rho_{\downarrow m\downarrow n} \right] + \frac{i}{2} \left[ \omega_c(n-m)\rho_{\downarrow m\downarrow n} + g \left( \sqrt{n+1}\rho_{\downarrow m+1\downarrow n} - \sqrt{m+1}\rho_{\downarrow m\downarrow n+1} \right) \right] + g \left( \sqrt{n+1}\rho_{\downarrow m+1\downarrow n} - \sqrt{m+1}\rho_{\downarrow m\downarrow n+1} \right),
$$
\[
\frac{d\rho_{mn}}{dt} = \kappa(\omega_c)[N(\omega_c) + 1]\left[\sqrt{(m+1)(n+1)}\rho_{(m+1)n+1} - \frac{1}{2}(m+n)\rho_{mn}\right]
\]
\[
+ \kappa(\omega_c)N(\omega_c)\left[\sqrt{mn}\rho_{mn-1n-1} - \frac{1}{2}(m+n+2)\rho_{mn}\right]
\]
\[
+ i\left[\omega_c(n-m) - \omega_0\right]\rho_{mn} + g(\sqrt{n}\rho_{mn-1} - \sqrt{m+1}\rho_{mn+1})
\]
\[
+ g(\sqrt{n+1}\rho_{mn} - \sqrt{m}\rho_{mn-1})\right],
\]
\[
\frac{d\rho_{mj}}{dt} = \kappa(\omega_c)[N(\omega_c) + 1]\left[\sqrt{(m+1)(n+1)}\rho_{mj+1n+1} - \frac{1}{2}(m+n)\rho_{mj}\right]
\]
\[
+ \kappa(\omega_c)N(\omega_c)\left[\sqrt{mn}\rho_{mn-1j-1} - \frac{1}{2}(m+n+2)\rho_{mj}\right]
\]
\[
+ i\left[\omega_c(n-m) + \omega_0\right]\rho_{mj} + g(\sqrt{n+1}\rho_{mj+1j} - \sqrt{m}\rho_{mj-1})
\]
\[
+ g(\sqrt{n}\rho_{mj} - \sqrt{m+1}\rho_{mj+1})\right].
\]

where \(\rho_{mn} = \langle m | \rho_S | n \rangle\). Corresponding component forms for the Jaynes–Cummings Hamiltonian (3.21) are obtained by dropping the last line from each of Eqs. (4.46) - (4.49). If \(g = 0\), the diagonal elements are independent of the off-diagonal ones, and the master equation for the diagonal elements can be written as
\[
\frac{d\rho_{mn}}{dt} = \kappa(\omega_c)[N(\omega_c) + 1]\left[(n+1)\rho_{mn+1} - np_{mn}\right] + \kappa(\omega_c)N(\omega_c)\left[n\rho_{n+1} - (n+1)p_{mn}\right].
\]
\[
\frac{d\rho_{mn}}{dt} = \kappa(\omega_c)[N(\omega_c) + 1]\left[(n+1)\rho_{mn+1} - np_{mn}\right] + \kappa(\omega_c)N(\omega_c)\left[n\rho_{n+1} - (n+1)p_{mn}\right],
\]
which are the same also in the interaction picture. For the off-diagonal element \(\rho_{mn}\) in the interaction picture, the master equation can be written as
\[
\frac{d\rho_{mn}}{dt} = \kappa(\omega_c)[N(\omega_c) + 1]\left[\sqrt{(m+1)(n+1)}\rho_{(m+1)n+1} - \frac{1}{2}(m+n)\rho_{mn}\right]
\]
\[
+ \kappa(\omega_c)N(\omega_c)\left[\sqrt{mn}\rho_{mn-1} - \frac{1}{2}(m+n+2)\rho_{mn}\right].
\]

Equations for other off-diagonal elements are obtained similarly.

Next we consider the eigenstate master equation. From now on our basis is the Hamiltonian eigenbasis \(| n \rangle\}. We start by using the definition \(\hat{S}_m = | n \rangle \langle m |\) and writing Eq. (4.34) (again neglecting the dephasing) as
\[
\frac{d\hat{S}_1}{dt} = \frac{1}{2} \sum_{\theta_{nm} > 0} \Gamma_{nm} \left[2|m\rangle \langle n| \hat{S}_1 + |n\rangle \langle m| \hat{S}_1 - \hat{S}_1 \langle n| \langle m|\right]
\]
\[
+ \frac{1}{2} \sum_{\theta_{nm} = 0} \Gamma_{nm} \left[2|m\rangle \langle n| \hat{S}_1 + |n\rangle \langle m| \hat{S}_1 - \hat{S}_1 \langle n| \langle m|\right].
\]

Since the \(k^{th}\) diagonal element of the density matrix is \(\rho_{kk} = \langle k| \hat{S}_1 | k \rangle\), we have that
\[
\frac{d\rho_{kk}}{dt} = \frac{1}{2} \sum_{\theta_{nm} > 0} \Gamma_{nm} \left[2|m\rangle \rho_{nm} \langle n| - |n\rangle \langle m| \rho_{kk} - \hat{S}_1 \langle n| \langle m|\right]
\]
\[
+ \frac{1}{2} \sum_{\theta_{nm} = 0} \Gamma_{nm} \left[2|m\rangle \rho_{nm} \langle n| - |n\rangle \langle m| \rho_{kk} - \hat{S}_1 \langle n| \langle m|\right].
\]

Calculating the diagonal matrix element, we obtain [8, 13, 43, 46]
\[
\langle k| \frac{d\hat{S}_1}{dt} | k \rangle = \langle k| \frac{d\rho_{kk}}{dt} = \frac{1}{2} \sum_{\theta_{nm} > 0} \Gamma_{nm} \left[2\langle k|m\rangle \rho_{nm} \langle m|k\rangle - \langle k|n\rangle \langle m|k| - \langle k| \hat{S}_1 | k \rangle \langle n|k\rangle\right]
\]
\[
+ \frac{1}{2} \sum_{\theta_{nm} = 0} \Gamma_{nm} \left[2\langle k|m\rangle \rho_{nm} \langle m|k\rangle - \langle k|n\rangle \langle m|k| - \langle k| \hat{S}_1 | k \rangle \langle n|k\rangle\right]
\]
\[
= \frac{1}{2} \sum_{m \neq k} \Gamma_{km} \langle k| - 2\rho_{kk} + \frac{1}{2} \sum_{m \neq k} \Gamma_{km} \left[2\rho_{nm}\right]
\]
\[
= \sum_{m \neq k} \Gamma_{km} \langle m| - \Gamma_{km} \rho_{kk}.
\]
which is the same also in the Schrödinger picture. This form is sometimes referred to as the Pauli master equation [4, 43], and it is always independent on the off-diagonal terms. Similar calculation for the off-diagonal element results in [8, 13, 46]

\[
\langle i \frac{d\rho_{ix}}{dt} | j \rangle = - \frac{1}{2} \sum_k (\Gamma_{i \rightarrow k} + \Gamma_{j \rightarrow k}) \rho_{ij}.
\] (4.59)

The solution for this can be written as

\[
\rho_{ij}(t) = \rho_{ij}(0) e^{-\frac{1}{2} \sum (\Gamma_{i \rightarrow k} + \Gamma_{j \rightarrow k}) t}.
\] (4.60)

It is clear that the off-diagonal elements are independent on other density matrix elements and that they decay when a sufficient amount of time has passed.

4.1.3. Applicability of the quantum optical master equation

When we derived the quantum optical master equation, we neglected the coupling between the qubit and the cavity. Thus, one could assume that in the limit \( g \rightarrow 0 \), the two master equations would be identical. Let us next consider this situation and check whether this indeed is the case.

If \( g = 0 \), transitions caused by the environment occur only between the eigenstates of the cavity. Thus, the state of the qubit is not changing. Therefore only the transitions

\[ \Gamma_{k+2 \rightarrow k} \quad \& \quad \Gamma_{k \rightarrow k+2}, \quad k = 0, 1, 2, \ldots \]

are non-zero, i.e. the state of the qubit is not changed and the number of quanta in the cavity is changed by \( \pm 1 \). Let us calculate their transition frequencies \( \omega_{k,k+2} \). First let \( k \) be even. We have

\[ \omega_{k,k+2} = \omega_{k+2} - \omega_k = (n+1)\omega_k - n\omega_k = \omega_k. \] (4.61)

Then let \( k \) be odd:

\[ \omega_{k,k+2} = [\omega_0 + (n+1)]\omega_k - [\omega_0 + n]\omega_k = \omega_k. \] (4.62)

We have shown that if there is no coupling between the qubit and the cavity, all transition frequencies are \( \omega_k \). We can then write the transition rates (4.33) with the definitions (4.42) and (4.43) as

\[ \Gamma_{k+2 \rightarrow k} = \kappa'(\omega_{k+2})[N(\omega_{k+2}) + 1]|\langle k| \hat{q} |k+2\rangle|^2 = \kappa'(\omega_k)[N(\omega_k) + 1](n+1), \] (4.63)

\[ \Gamma_{k \rightarrow k+2} = \kappa'(\omega_{k+2})N(\omega_{k+2})|\langle k+2| \hat{q} |k\rangle|^2 = \kappa'(\omega_k)N(\omega_k)(n+1), \] (4.64)

where \( n \) is the number of quanta in the cavity. Using these we can write Eq. (4.58) as

\[ \frac{d\rho_{kk}}{dt} = \Gamma_{k+2 \rightarrow k} \rho_{k+2,k+2} + \Gamma_{k \rightarrow k+2} \rho_{k-2,k-2} - (\Gamma_{k \rightarrow k+2} + \Gamma_{k \rightarrow k-2}) \rho_{kk}, \] (4.65)

which for \( \rho_{\gamma\gamma_n} \) results in:

\[ \frac{d\rho_{\gamma\gamma_n}}{dt} = \Gamma_{\gamma+1 \rightarrow \gamma_n} \rho_{\gamma+1,\gamma_n+1} + \Gamma_{\gamma_n-1 \rightarrow \gamma_n} \rho_{\gamma_n-1,\gamma_n-1} - (\Gamma_{\gamma_n \rightarrow \gamma_{n+1}} + \Gamma_{\gamma_n \rightarrow \gamma_{n-1}}) \rho_{\gamma\gamma_n} \] (4.66)

\[ = \kappa'(\omega_k)[N(\omega_k) + 1]|(n+1)\rho_{\gamma+1,\gamma_n+1} - n\rho_{\gamma\gamma_n}] + \kappa'(\omega_k)N(\omega_k)n\rho_{\gamma\gamma_n} - (n+1)\rho_{\gamma\gamma_n}. \] (4.67)

For \( \rho_{\gamma_n\gamma_n} \) we obtain similarly:

\[ \frac{d\rho_{\gamma_n\gamma_n}}{dt} = \kappa'(\omega_k)[N(\omega_k) + 1]|(n+1)\rho_{\gamma_n+1,\gamma_n+1} - n\rho_{\gamma_n\gamma_n}] + \kappa'(\omega_k)N(\omega_k)n\rho_{\gamma_n\gamma_n} - (n+1)\rho_{\gamma_n\gamma_n}. \] (4.68)

These are exactly the same as Eqs. (4.50) and (4.51), so both master equations give the same time evolution for the diagonal elements if \( g = 0 \). Let us then consider the off-diagonal element \( \rho_{\gamma\gamma_n} \). Using Eq. (4.59) we obtain

\[ \frac{d\rho_{\gamma\gamma_n}}{dt} = -\frac{1}{2}\rho_{\gamma\gamma_n} \left[ \Gamma_{\gamma+1 \rightarrow \gamma_n+1} + \Gamma_{\gamma_n \rightarrow \gamma_n-1} + \Gamma_{\gamma_n \rightarrow \gamma_n-1} + \Gamma_{\gamma_n \rightarrow \gamma_n+1} \right] \] (4.69)

\[ = -\frac{1}{2}\rho_{\gamma\gamma_n} \left[ (m+1)|\kappa'(\omega_k)[N(\omega_k) + 1] + (n+1)|\kappa'(\omega_k)N(\omega_k) + n\kappa'(\omega_k)N(\omega_k) + 1 \right]. \] (4.70)
which has the solution
\[ \rho(t) = \rho(0) e^{-\omega t[N(m+n+1)+(m+n)/2]}. \] (4.71)

Other off-diagonal elements can be treated similarly. By comparing Eqs. (4.52) and (4.70), we notice that they are not equal. In the eigenstate master equation the off-diagonals evolve independently, whereas in the quantum optical master equation they are dependent on the elements corresponding to cavity states with \( \pm 1 \) quanta. The dependence on the other terms comes from the terms \( \hat{a}_s \hat{a}^\dagger \) and \( \hat{a}^\dagger \hat{a}_s \). These terms are produced by the terms \( \hat{q}(t) \hat{p}_{s;l} \hat{q}(t - \tau) \) and \( \hat{q}(t - \tau) \hat{p}_{s;l} \hat{q}(t) \) in Eq. (4.15). When we derived the eigenstate master equation, we made the secular approximation and discarded terms of the form \( \hat{q}_{lm} \hat{p}_{s;l} \hat{q}_{lm} e^{-2i \omega_{om} t} \) and \( \hat{q}_{lm} \hat{p}_{s;l} \hat{q}_{lm} e^{2i \omega_{om} t} \), but we simultaneously also discarded hermitian conjugate terms with different indices, e.g. \( \hat{q}_{lm} \hat{p}_{s;l} \hat{q}_{lm} e^{i(\omega_{om} - \omega_{om}) t} \). These terms are rapidly oscillating, but if \( g = 0 \), all transitions energies are \( \omega_{om} \). Therefore the exponent factors causing the oscillations vanish in the hermitian conjugate terms with different indices, and discarding them in the secular approximation is no longer justified. It turns out that these terms indeed cause the off-diagonal elements of the density matrix to depend on other off-diagonal elements: \( \hat{r}_{nm} \hat{p}_{s;l} \hat{r}_{nm} = |n\rangle \langle m| \hat{p}_{s;l} |l\rangle \langle k| = \rho_{ml} |n\rangle \langle k| \). This does not happen with the terms \( \hat{q}(t) \hat{q}(t - \tau) \hat{p}_{s;l} \) and \( \hat{p}_{s;l} \hat{q}(t - \tau) \hat{q}(t) \), since the only terms left from the inner products are now terms with the same indices, e.g. \( \hat{r}_{nm} \hat{p}_{s;l} \hat{r}_{nm} = |n\rangle \langle m| \langle k| \neq 0 \) if and only if \( m = l \). It therefore seems that the eigenstate master equation can be improved further by taking into account the terms with different indices.

### 4.2. Stochastic Liouville–von Neumann equation

A lot of assumptions and approximations were made when we derived the Lindblad master equations. Using path integral formalism we derive here a formally exact equation for the time evolution of the reduced density matrix. This equation is the stochastic Liouville–von Neumann equation.

#### 4.2.1. Derivation

We again assume that the studied quantum system is coupled bilinearly to the bosonic bath in thermal equilibrium. In this case the reduced density operator in the path integral formalism can be written as [6, 44]

\[
\rho_S(q,t) = \int dq'_1 \int dq'_2 D[q_1] D[q_2] \exp \left\{ i \frac{\hbar}{\omega} (S_S[q_1] - S_S[q_2]) \right\} F[q_1 - q, q_1 + q_2] \rho_S(q_1, q'_1, t),
\] (4.72)

where \( S_S[q] \) is the classical action functional of the system under study, \( \rho_S(q_1, q'_1, t) \) the initial reduced density operator and \( F[x, r] \) is the Feynman–Vernon influence functional which describes the effect of the environment to the system dynamics [5, 6]. It is defined as

\[
F[x, r] = \exp \left\{ -\frac{i}{\hbar} \Phi[x, r] \right\},
\] (4.73)

where

\[
\Phi[x, r] = \frac{1}{\hbar} \int_0^t dt' \int_0^t dt'' s(t') \left( L_R(t' - t'') s(t'') + i L_4(t' - t'') r(t'') \right) + \frac{i \mu}{\hbar} \int_0^t dt' s(t') r(t').
\] (4.74)

Here \( L_R \) and \( L_4 \) are the real and imaginary parts of the environmental correlation function (3.72), respectively. Coefficient \( \mu \) is a constant potential renormalization term, which is defined by the imaginary part of the correlation function [5, 6, 10]. Using the second power in the Drude model we obtain

\[
\mu = -\frac{1}{\hbar} \int_0^{\infty} dt L_4(t) = \frac{\eta \omega_0^3}{4} \int_0^{\infty} dt e^{-\omega_0 t} = \frac{\eta \omega_0^3}{4},
\] (4.75)

where we used Eq. (3.90). We can include the potential term in the other integral in Eq. (4.74) by recognizing that [5, 6]

\[
\int_0^t dt' s(t') r(t') = \int_0^t dt' \int_0^t dt'' s(t') \delta(t' - t'') r(t'').
\] (4.76)

With this, Eq. (4.74) can be written as

\[
\Phi[x, r] = \frac{1}{\hbar} \int_0^t dt' \int_0^t dt'' s(t') \left\{ L_R(t' - t'') s(t'') + \left[ i L_4(t' - t'') + i \mu \delta(t' - t'') \right] r(t'') \right\}.
\] (4.77)
We can further write Eq. (4.73) as a stochastic average of a Gaussian functional $W[\zeta, v]$ using two stochastic complex noise terms $\zeta(t)$ and $v(t)$ [6, 44]:

$$F[s, r] = \int D^2[\zeta] \int D^2[v] W[\zeta, v] \exp \left\{ \frac{i}{\hbar} \int_{t_0}^t dt' [\zeta(t') + v(t')r(t')] \right\}. \quad (4.78)$$

These complex noise terms obey the correlations [5, 6, 8, 9, 10, 44]

$$\langle \zeta(t) \zeta(t') \rangle = L_R(t - t'), \quad (4.79)$$
$$\langle \zeta(t)v(t') \rangle = i\Theta(t - t')L_4(t - t') + i\mu \delta(t - t') = -i\chi(t - t') + i\mu \delta(t - t'), \quad (4.80)$$
$$\langle v(t)v(t') \rangle = 0. \quad (4.81)$$

where $\Theta(t - t')$ is the Heaviside step function as defined in Eq. (3.79). Here the averages $\langle \ldots \rangle$ are stochastic averages over Gaussian processes [44]. Using now the definitions $s = q_1 - q_2$ and $r = q_1 + q_2$, we obtain

$$F[q_1 - q_2, q_1 + q_2] = \int D^2[\zeta] \int D^2[v] W[\zeta, v] \exp \left\{ \frac{i}{\hbar} \int_{t_0}^t dt' [\zeta(t') + v(t')q_1(t') - [\zeta(t') - v(t')]q_2(t')] \right\}. \quad (4.82)$$

The entire path integral Eq. (4.72) is then written as

$$\hat{\rho}_S(q_1, q_2; t) = \int dq_1 \int dq_2 \int_{q_1}^{q_2} D[q_1] \int_{q_2}^{q_1} D[q_2] \int D^2[\zeta] \int D^2[v]$$
$$\times W[\zeta, v] \exp \left\{ \frac{i}{\hbar} \left( S_S[q_1] - S_S[q_2] \right) + \frac{i}{\hbar} \int_{t_0}^t dt' [\zeta(t') + v(t')q_1(t') - [\zeta(t') - v(t')]q_2(t')] \right\} \times \hat{\rho}_S(q_1, q_2; t_0). \quad (4.83)$$

From this we identify two stochastic propagators [5]:

$$G_1(q_1, q_2; t) = \int_{q_1}^{q_2} D[q_1] \int D[\zeta] \int D[v] \exp \left\{ \frac{i}{\hbar} S_S[q_1] + \frac{i}{\hbar} \int_{t_0}^t dt' [\zeta(t') + v(t')q_1(t')] \right\}, \quad (4.84)$$
$$G_2(q_1, q_2; t) = \int_{q_2}^{q_1} D[q_2] \int D[\zeta] \int D[v] \exp \left\{ -\frac{i}{\hbar} S_S[q_2] - \frac{i}{\hbar} \int_{t_0}^t dt' [\zeta(t') - v(t')q_2(t')] \right\}. \quad (4.85)$$

Here the integral terms in the exponents can be interpreted as time dependent potentials. From these we can recover the corresponding Hamiltonian operators, which allows us to write two Schrödinger equations for the states $|\psi_1\rangle$ and $|\psi_2\rangle$ [5]:

$$\frac{i\hbar}{\hbar} \frac{d|\psi_1\rangle}{dt} = \hat{H}_S |\psi_1\rangle - \zeta(t)\hat{q} |\psi_1\rangle - v(t)\hat{q} |\psi_1\rangle, \quad (4.86)$$
$$\frac{i\hbar}{\hbar} \frac{d|\psi_2\rangle}{dt} = \hat{H}_S |\psi_2\rangle - \zeta(t)\hat{q} |\psi_2\rangle + v^*(t)\hat{q} |\psi_2\rangle. \quad (4.87)$$

If we then define the reduced density operator as $\hat{\rho}_S = |\psi_1\rangle \langle \psi_2|$, we obtain

$$\frac{i\hbar}{\hbar} \frac{d\hat{\rho}_S(t)}{dt} = \frac{i}{\hbar} \frac{d|\psi_1\rangle}{dt} \langle \psi_2| + \frac{i}{\hbar} |\psi_1\rangle \frac{d|\psi_2\rangle}{dt}, \quad (4.88)$$
$$= \hat{H}_S\hat{\rho}_S(t) - \zeta(t)\hat{q}\hat{\rho}_S(t) - v(t)\hat{q}\hat{\rho}_S(t) - \hat{\rho}_S(t)\hat{H}_S + \zeta(t)\hat{\rho}_S(t)\hat{q} - v(t)\hat{\rho}_S(t)\hat{q}, \quad (4.89)$$
$$= [\hat{H}_S, \hat{\rho}_S(t)] - \zeta(t)\hat{q}\hat{\rho}_S(t) - v(t)\hat{q}\hat{\rho}_S(t) - \zeta(t)\hat{\rho}_S(t)\hat{q}, \quad (4.90)$$

which is the stochastic Liouville–von Neumann equation [5, 6, 49]. If we did not combine the constant potential term with the rest of the terms in Eq. (4.77), we would have obtained an additional term in the stochastic Liouville–von Neumann equation [5, 6, 8, 9, 10, 44, 49]:

$$\frac{i\hbar}{\hbar} \frac{d\hat{\rho}_S(t)}{dt} = [\hat{H}_S, \hat{\rho}_S(t)] - \zeta(t)\hat{q}\hat{\rho}_S(t) - v(t)\hat{q}\hat{\rho}_S(t) + \mu[\hat{q}^2, \hat{\rho}_S(t)]. \quad (4.91)$$

This would also have produced a cross-correlator (4.80) without the delta function:

$$\langle \zeta(t)v(t') \rangle = -i\chi(t - t'). \quad (4.92)$$

In this case, however, the spectrum of complex noise terms lies between the Drude cutoff frequencies $-\omega_D$ and $\omega_D$. The system frequencies are also located within this interval. This causes the complex noise terms to drive
the system in resonance, which effectively causes the numerical simulations to become unstable at some critical
time \( t_c \). In the case of the Eq. (4.90) with correlations (4.79) - (4.81), the complex noise spectrum has a gap in the
interval \([\theta_0, \theta_2]\). This reduces the resonant driving considerably and increases the critical time significantly,
allowing longer simulation timescales. [5, 6, 49]

In this thesis we use Eq. (4.90) and noise correlations (4.79) - (4.81) to solve the system dynamics.

4.2.2. Complex noises

Generation of the noise terms obeying correlations (4.79) - (4.81) goes as follows. We first assume, that we
can split \( \zeta \)-noise into purely real and complex parts: \( \zeta(t) = \zeta_R(t) + i\zeta_C(t) \). Complex part can further be split
into real and imaginary parts: \( \zeta_C(t) = \zeta_{CR}(t) + i\zeta_{CI}(t) \). For the \( \nu \)-noise, we split it into real and imaginary parts:
\( \nu(t) = \nu_R(t) + i\nu_I(t) \). We then have following correlations for the noise terms [5, 10]:

\[
\langle \zeta_R(t)\zeta_R(t') \rangle = L_R(t - t'), \\
\langle \zeta_C(t)\zeta_C(t') \rangle = 0, \\
\langle \zeta_R(t)\nu(t') \rangle = 0, \\
\langle \zeta_C(t)\nu(t') \rangle = -i\xi(t - t') + i\mu(t - t'), \\
\langle \nu(t)\nu(t') \rangle = 0.
\] (4.93)

(4.94)

(4.95)

(4.96)

(4.97)

We can now generate noises with these properties by first generating Gaussian white noise (with zero mean and
unit standard deviation) with the autocorrelation [5, 44]

\[
\langle x(t)x(t') \rangle = \delta(t - t'),
\] (4.98)

and then filtering it with a proper window function.

Let us start with \( \zeta_R(t) \). We write [5, 10]

\[
\zeta_R(t) = \int_{-\infty}^{\infty} dt' G(t - t')x(t'),
\] (4.99)

where \( G(t) \) is a real valued window function. The correlation is then

\[
\langle \zeta_R(t)\zeta_R(t') \rangle = \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau' G(t - \tau)G(t' - \tau')\langle x(\tau)x(\tau') \rangle.
\] (4.100)

By using the Eq. (4.98), we obtain

\[
L_R(t - t') = d\tau \int_{-\infty}^{\infty} d\tau' G(t - \tau)G(t' - \tau).
\] (4.101)

In the next step we need the Fourier transforms

\[
\tilde{L}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} L(t),
\] (4.102)

\[
\tilde{G}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G(t),
\] (4.103)

\[
L(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{L}(\omega),
\] (4.104)

\[
G(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{G}(\omega).
\] (4.105)

We write Eq. (4.101) in terms of inverse Fourier transforms (4.104) and (4.105) and obtain [10]

\[
\text{Re} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')} \tilde{L}(\omega) = \frac{1}{2\pi} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\tau e^{-i\omega(t-t')}e^{-i\omega'(t'-t')} \tilde{G}(\omega)\tilde{G}(\omega')
\] (4.106)

\[
= \frac{1}{2\pi} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\tau e^{i\omega(t+t')}e^{-i\omega(t+t')} \tilde{G}(\omega)\tilde{G}(\omega')
\] (4.107)

\[
= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \delta(\omega + \omega')e^{-i\omega(t+t')} \tilde{G}(\omega)\tilde{G}(\omega')
\] (4.108)

\[
= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')} \tilde{G}(\omega)\tilde{G}(-\omega).
\] (4.109)
Because the window function \(G(t)\) is real, its Fourier transform has property \(G^*(\omega) = \tilde{G}(-\omega)\). In addition, by using Eq. (3.72) we see that \(L(-t) = L^*(t)\). This implies that \(\tilde{L}(\omega)\) is real. The environmental correlation function has the following symmetry relations [10]:

\[
\begin{align*}
L_R^R(t) &= L_R(-t), \\
L_I^I(t) &= -L_I(-t).
\end{align*}
\]

Thus, \(\tilde{L}_R(\omega)\) and \(\tilde{L}_I(\omega)\) are real. Also because \(L_R(t)\) is real, \(\tilde{L}_R(\omega) = \bar{L}_R(\omega)\), which means that \(\tilde{L}_I(\omega)\) is an even function. Similarly \(i\tilde{L}_I(\omega)\) is an odd function. Therefore odd part vanishes in the real part of the Fourier transform, and we are left with [10]:

\[
\Re \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')}L(\omega) = \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')}|\tilde{G}(\omega)|^2
\]

\[
\implies |	ilde{G}(\omega)|^2 = L_R(\omega).
\]

Using Eq. (3.98), we can write

\[
\tilde{G}(\omega) = \sqrt{h\coth(\beta\hbar\omega/2)}J(\omega).
\]

We have now obtained an analytic form for the Fourier transform of the window function required for the computation of the \(\xi_R(t)\). We can now write

\[
\xi_R(t) = \int_{-\infty}^{\infty} dt' \bar{G}(t-t')x(t'),
\]

\[
= \frac{1}{2\pi} \frac{1}{2\pi} \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' e^{-i\omega(t-t')} \bar{G}(\omega)e^{-i\omega'(t')} \tilde{x}(\omega'),
\]

\[
= \frac{1}{2\pi} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \tilde{G}(\omega)\tilde{x}(\omega) e^{-i\omega(t-t')} \int_{-\infty}^{\infty} dt' e^{-i\omega'(t-t')},
\]

\[
= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega \tilde{G}(\omega)\tilde{x}(\omega') e^{-i\omega \delta(\omega - \omega')},
\]

\[
= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega \delta} \tilde{G}(\omega)\tilde{x}(\omega).
\]

Let us proceed similarly with the remaining noise terms. We write

\[
\xi_C^R(t) = \int_{-\infty}^{\infty} dt' W_{\xi_C}^R(t-t')z_1(t'),
\]

\[
\xi_C^I(t) = \int_{-\infty}^{\infty} dt' W_{\xi_C}^I(t-t')z_2(t'),
\]

\[
\nu^R(t) = \int_{-\infty}^{\infty} dt' W_{\nu}^R(t-t')z_3(t'),
\]

\[
\nu^I(t) = \int_{-\infty}^{\infty} dt' W_{\nu}^I(t-t')z_4(t'),
\]

where the \(W\)'s are the corresponding window functions and \(z_i\)'s are the Gaussian white noises. Equations (4.94) and (4.97) are fulfilled, if \(W_{\xi_C}^R = W_{\xi_C}^I \equiv W_{\xi_C}\) and \(W_{\nu}^R = W_{\nu}^I \equiv W_{\nu}\) [10]. From the cross-correlator (4.96) we obtain

\[
\langle \xi_C(t)\nu(t') \rangle = \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau' W_{\xi_C}(t-\tau)W_{\nu}(t'-\tau')
\]

\[
\times \{\langle z_1(\tau)z_3(\tau') \rangle - \langle z_1(\tau)z_4(\tau') \rangle + i\langle z_1(\tau)z_4(\tau') \rangle + \langle z_2(\tau)z_3(\tau') \rangle\},
\]

\[
= 2i \int_{-\infty}^{\infty} d\tau W_{\xi_C}(t-\tau)W_{\nu}(t'-\tau),
\]

\[
= -i\chi(t-t') + i\mu \delta(t-t'),
\]

where we have chosen \(z_1(t) = z_2(t)\) and \(z_2(t) = z_3(t)\). We have also used the autocorrelation property of the Gaussian white noise (Eq. (4.98)). Let us then again use the inverse Fourier transform and find out the relations
Because our window functions are real valued in the time domain, in frequency domain they have the property

\[ \mathcal{W}_c(\omega) = \mathcal{W}_c^*(\omega) \]

Therefore we obtain

\[ \mathcal{W}_c(\omega) = \mathcal{W}_c^*(\omega) = -\frac{1}{2} [\mathcal{X}(\omega) - \mu]. \]

Because \( \mathcal{X}(\omega) \) is complex valued, we can choose our window functions to be \( \mathcal{W}_c(\omega) = -\mathcal{W}_c^*(\omega) \equiv \mathcal{W}(\omega) \) [10]. Therefore

\[ \mathcal{W}(\omega) = \left[ \frac{1}{2} \mathcal{X}(\omega) \right]^{1/2}. \]

If we had used the cross-correlator without delta function (Eq. (4.92)), we would have obtained [10]

\[ \mathcal{W}(\omega) = \left[ \frac{1}{2} \mathcal{X}(\omega) \right]^{1/2}. \]

It turns out that we can obtain an analytic form for \( \mathcal{X}(\omega) \). We start with the Fourier transform and obtain

\[ \mathcal{X}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \mathcal{X}(\tau) = -\int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \Theta(\tau) L_3(\tau) = \frac{\eta \alpha_1^2 \hbar}{4} \int_{0}^{\infty} d\tau e^{i\omega\tau} \tau e^{-i\omega_0 \tau}, \]

where we have used the analytic form for the \( L_3 \), which was given in Eq. (3.90). We notice that this is just the Laplace transform of \( \tau e^{i\omega\tau} \). We obtain

\[ \mathcal{X}(\omega) = \frac{\eta \alpha_1^2 \hbar}{4} \frac{1}{(i\omega - i\omega_0)^2}. \]

Let us simplify this:

\[ \frac{1}{(i\omega - i\omega_0)^2} = \frac{1 - \omega^2/\omega_0^2}{\omega_0^2(1 + \omega^2/\omega_0^2)} + \frac{2i\omega}{\omega_0^2(1 + \omega^2/\omega_0^2)^2}. \]

Therefore

\[ \mathcal{X}(\omega) = \frac{\hbar \omega_0}{4\omega} J(\omega) \left( 1 - \frac{\omega^2}{\omega_0^2} \right) + \frac{\hbar}{2} J(\omega). \]

We now have analytic forms for both \( \tilde{G}(\omega) \) and \( \tilde{W}(\omega) \), which we need in order to calculate the noises \( \zeta(t) \) and \( \nu(t) \) from three Gaussian white noises \( x(t) \), \( z_1(t) \) and \( z_2(t) \):

\[ \zeta_R(t) = \int_{-\infty}^{\infty} dt' G(t - t') x(t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{G}(\omega) \tilde{x}(\omega), \]

\[ \zeta_I(t) = \int_{-\infty}^{\infty} dt' W(t - t') z_1(t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{W}(\omega) \tilde{z}_1(\omega), \]

\[ \nu_R(t) = \int_{-\infty}^{\infty} dt' W(t - t') z_2(t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{W}(\omega) \tilde{z}_2(\omega), \]

\[ \nu_I(t) = \int_{-\infty}^{\infty} dt' W(t - t') z_1(t') = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{W}(\omega) \tilde{z}_1(\omega), \]

\[ \zeta_R(t) = \int_{-\infty}^{\infty} dt' W(t - t') z_2(t') = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{W}(\omega) \tilde{z}_2(\omega), \]

\[ \nu_I(t) = \int_{-\infty}^{\infty} dt' W(t - t') z_1(t') = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{W}(\omega) \tilde{z}_1(\omega), \]

\[ \zeta_I(t) = \int_{-\infty}^{\infty} dt' W(t - t') z_2(t') = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{W}(\omega) \tilde{z}_2(\omega), \]

\[ \nu_R(t) = \int_{-\infty}^{\infty} dt' W(t - t') z_1(t') = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{W}(\omega) \tilde{z}_1(\omega), \]
where window functions for the second power in the Drude model are

\[
G(\omega) = \frac{\hbar \eta \omega \coth(\beta \hbar \omega / 2)}{(1 + \omega^2 / \omega_0^2)N},
\]

(4.143)

\[
W(\omega) = \frac{\omega_0 \eta}{8} \left[ \frac{\hbar(1 - \omega^2 / \omega_0^2)}{(1 + \omega^2 / \omega_0^2)^2} - 1 \right] + \frac{\hbar \eta \omega}{4(1 + \omega^2 / \omega_0^2)}N,
\]

(4.144)

where in Eq. (4.144) we have used Eq. (4.75) for the potential term.

### 4.2.3. Component form of the stochastic Liouville–von Neumann equation

Let us then for completeness present the component form of the stochastic Liouville–von Neumann equation (4.90) in the product basis \(\{|\uparrow n\rangle\}\) with the Rabi Hamiltonian. The equations governing the time evolution of the density matrix elements can be written as

\[
\frac{d\rho_{\uparrow\uparrow}}{dt} = \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m} \rho_{\uparrow\downarrow} + \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m + 1} \rho_{\downarrow\uparrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m + 1} \rho_{\uparrow\downarrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m} \rho_{\downarrow\uparrow} + g \left( \sqrt{m} \rho_{\uparrow\downarrow} - \sqrt{m + 1} \rho_{\downarrow\uparrow} \right)\]

(4.145)

\[
\frac{d\rho_{\downarrow\downarrow}}{dt} = \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m} \rho_{\downarrow\uparrow} + \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m + 1} \rho_{\uparrow\downarrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m + 1} \rho_{\downarrow\uparrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m} \rho_{\uparrow\downarrow} + g \left( \sqrt{m + 1} \rho_{\uparrow\downarrow} - \sqrt{m} \rho_{\downarrow\uparrow} \right)\]

(4.146)

\[
\frac{d\rho_{\uparrow\downarrow}}{dt} = \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m + 1} \rho_{\uparrow\downarrow} + \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m + 1} \rho_{\downarrow\uparrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m + 1} \rho_{\downarrow\uparrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m} \rho_{\uparrow\downarrow} + g \left( \sqrt{m + 1} \rho_{\uparrow\downarrow} - \sqrt{m} \rho_{\downarrow\uparrow} \right)\]

(4.147)

\[
\frac{d\rho_{\downarrow\uparrow}}{dt} = \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m + 1} \rho_{\downarrow\uparrow} + \frac{i}{\hbar} \left[ \zeta(t) + v(t) \right] \sqrt{m + 1} \rho_{\uparrow\downarrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m + 1} \rho_{\downarrow\uparrow} + \frac{i}{\hbar} \left[ \zeta(t) - v(t) \right] \sqrt{m} \rho_{\uparrow\downarrow} + g \left( \sqrt{m + 1} \rho_{\downarrow\uparrow} - \sqrt{m} \rho_{\uparrow\downarrow} \right)\]

(4.148)

Here, again, the equations with the Jaynes–Cummings Hamiltonian are obtained from Eqs. (4.145) - (4.148) by dropping the last lines. From these equations one can observe that the stochastic Liouville–von Neumann equation is more complicated than the master equations, since, in addition to the stochastic complex noises, the diagonal and off-diagonal terms depend heavily on each other.

### 4.3. Steady state solutions

If a small quantum system is coupled to a reservoir, there is exchange of energy between the small system and the reservoir. The master equations govern these occurrences by the dissipation and absorption terms, and the stochastic
The steady state density operator is then \[ \rho_{ss}^{\text{eq}} = \frac{1}{Z} e^{-\beta \hat{H}}, \] (4.149)

where \( Z \) is the partition function determining the normalization of the system:
\[ Z = \text{Tr} e^{-\beta \hat{H}}. \] (4.150)

The occupation probability of the \( k \)-th eigenstate of the Hamiltonian \( \hat{H} \) in the equilibrium is thus given by
\[ p_k = \frac{\rho_{ss}^{\text{eq}}}{\sum e^{-\beta \hbar \omega_k}}. \] (4.151)

Let us first show that this holds for the Pauli master equation (4.58). For the average number of quanta we have
\[ N(\omega) + 1 = \frac{e^{\beta \hbar \omega}}{e^{\beta \hbar \omega} - 1} = e^{\beta \hbar \omega} N(\omega), \] (4.152)

Because the operator \( \hat{q} \) is Hermitian, we have
\[ \langle k | \hat{q} | m \rangle |^2 = \langle m | \hat{q} | k \rangle |^2. \] (4.153)

For transitions \( \omega_{mk} > 0 \) we can then write
\[ \Gamma_{k \rightarrow m} = \langle m | \hat{q} | k \rangle |^2 \kappa(\omega_{mk})N(\omega_{mk}) + 1 \rangle \langle k | \hat{q} | m \rangle |^2 \kappa(\omega_{mk})N(\omega_{mk}) e^{\beta \hbar \omega_{mk}} = e^{\beta \hbar \omega_{mk}} \Gamma_{m \rightarrow k}. \] (4.154)

With this we can write the Pauli master equation (4.58) as
\[ \frac{d\rho_{kk}}{dt} = \sum_{m \neq k} \left[ \Gamma_{m \rightarrow k} \rho_{mm} - \Gamma_{k \rightarrow m} \rho_{kk} \right] = \sum_{m \neq k} \Gamma_{m \rightarrow k} \left[ \rho_{mm} - e^{\beta \hbar \omega_{mk}} \rho_{kk} \right]. \] (4.155)

In the equilibrium \( \frac{d\rho_{kk}}{dt} = 0 \). With this and Eq. (4.151), Eq. (4.155) is transformed into
\[ 0 = \sum_{m \neq k} \Gamma_{m \rightarrow k} \left[ e^{-\beta \hbar \omega_{mk}} - e^{\beta \hbar (\omega_k - \omega_m)} \right] e^{-\beta \hbar \omega} = \sum_{m \neq k} \Gamma_{m \rightarrow k} \left[ e^{-\beta \hbar \omega - \beta \hbar \omega_{mk}} - e^{-\beta \hbar \omega_{mk}} \right] = 0, \] (4.156)

thus showing that the steady state of the eigenstate master equation is indeed given by the Gibbs distribution (4.149).

For the quantum optical master equation, however, this is not the case [11]. Let us instead consider the uncoupled Hamiltonian in resonance (\( \omega_k = \omega_0 + \omega \))
\[ \hat{H}_0 = \hbar \omega (\hat{a}^\dagger \hat{a} + \sigma_+ \sigma_-). \] (4.157)

The steady state density operator is then [11]
\[ \rho_{ss}^{\text{eq}} = \frac{1}{Z} e^{-\beta \hat{H}_0}, \] (4.158)

which is diagonal in the product basis \([\uparrow \downarrow n]\). To show that this indeed is the steady state solution, consider the state \([\downarrow n]\), which has energy \( n \hbar \omega \). From Eq. (4.47) we obtain
\[ 0 = \kappa(N + 1)[(n + 1) \rho_{\downarrow \uparrow +1,\downarrow n + 1}^{\text{eq}} - n \rho_{\downarrow \downarrow n,\downarrow n}^{\text{eq}}] + \kappa N [n \rho_{\downarrow \downarrow n - 1,\downarrow n - 1}^{\text{eq}} - (n + 1) \rho_{\downarrow \downarrow n,\downarrow n}^{\text{eq}}], \] (4.159)
\[ = \frac{e^{\beta \hbar \omega}}{e^{\beta \hbar \omega} - 1} [(n + 1) e^{-\beta \hbar \omega} - n] + \frac{1}{e^{\beta \hbar \omega} - 1} [n e^{\beta \hbar \omega} - (n + 1)], \] (4.160)
\[ = \frac{n + 1}{e^{\beta \hbar \omega} - 1} - \frac{n e^{\beta \hbar \omega}}{e^{\beta \hbar \omega} - 1} + \frac{n e^{\beta \hbar \omega}}{e^{\beta \hbar \omega} - 1} - \frac{n + 1}{e^{\beta \hbar \omega} - 1} = 0. \] (4.161)
In a similar way one can treat the state $|\uparrow n\rangle$ with energy $(n + 1)\hbar \omega$. Thus, (4.158) is the steady state of the quantum optical master equation. Numerical results suggest that this holds only for the Jaynes–Cummings Hamiltonian. For the Rabi Hamiltonian no analytical equilibrium distribution is known for the author. Numerical results further suggest that the steady state of the quantum optical master equation is independent on $g$ and $\omega_0$: even in off-resonance the steady state is given by the Gibbs distribution with the resonant Hamiltonian (4.157). This happens because the dissipators in the quantum optical master equation depend only on $\omega_c$ and the temperature $T$.

Comparison of the distributions (4.149) and (4.158) is shown in Figure 3 for the resonant Jaynes–Cummings Hamiltonian. One notices that the differences between the steady states of the excited states grow with increasing $g$. The differences in the ground state grow much slower. The excited states are paired, and the quantum optical master equation suggests that in the steady state these paired states have the same occupation probabilities. The eigenstate master equation, on the other hand, shows that their steady state occupation probabilities are equal distance higher and lower than the values suggested by the quantum optical master equation. The difference becomes non negligible already at very weak qubit-cavity coupling ($g \approx 0.02$). The discussion in Section 3 suggests that the Jaynes–Cummings Hamiltonian is valid in this region.

In the case of the stochastic Liouville–von Neumann equation (4.90), one is likely to observe differences from the Gibbs distribution, especially with stronger environmental couplings.

![Figure 3: The steady state occupation probabilities for the eigenstate master equation (solid line) and the quantum optical master equation (dashed line) for the resonant qubit-cavity system as a function of coupling $g$. Parameters are: $\omega_c = \omega_0 = 1$.](image_url)
5. Numerical methods and simulations

In this section we discuss the numerical methods we have used for solving the master equations and the stochastic Liouville–von Neumann equation, but first let us briefly recall the equations.

The quantum optical master equation is written as

\[
\frac{d\hat{\rho}_S(t)}{dt} = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S(t)] + \frac{\kappa(\omega_k)}{2} [N(\omega_k) + 1] \left[ 2\hat{a}^\dagger \hat{\rho}_S(t) \hat{a}^\dagger - \hat{a}^\dagger \hat{a} \hat{\rho}_S(t) \right]
\]  

(5.1)

and the eigenstate master equation as

\[
\frac{d\hat{\rho}_S(t)}{dt} = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S(t)] + \frac{1}{7} \sum_{\omega_{nm}} \kappa(\omega_{nm}) [N(\omega_{nm}) + 1] \left[ 2\hat{a}_{nm}^\dagger \hat{\rho}_S(t) \hat{a}_{nm} - \hat{a}_{nm}^\dagger \hat{a}_{nm} \hat{\rho}_S(t) \right]
\]  

(5.2)

and also in a matrix-vector form as

\[
\frac{d\hat{\rho}(t)}{dt} = \mathbf{A}(t)\hat{\rho}(t) + \mathbf{f}(t)\mathbf{1}.
\]  

(5.3)

The stochastic Liouville–von Neumann equation is given by

\[
\frac{d\hat{\rho}_S(t)}{dt} = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S(t)] + \frac{i}{\hbar} \zeta(t)[\hat{q}, \hat{\rho}_S(t)] + \frac{i}{\hbar} v(t)[\hat{q}, \hat{\rho}_S(t)].
\]  

(5.4)

These three equations govern the time evolution of the reduced density operator \(\hat{\rho}_S(t)\). For the qubit-cavity system this operator is an infinite-dimensional matrix. For the numerical purposes, we have to truncate it to a finite matrix. Thus, the above equations effectively form sets of coupled differential equations. In our case, the Hamiltonians (3.11) and (3.21) and the coupling between the system and the reservoir are time-independent. Thus, the corresponding master equations (5.1) and (5.2) are also time-independent. The stochastic Liouville–von Neumann equation (5.3), however, contains time-dependent terms, namely the noises \(\zeta(t)\) and \(v(t)\). Therefore, we have to solve both time-independent and time-dependent sets of differential equations, which in general can be written as

\[
\begin{align*}
\gamma_0(t) &= f_0[t, \gamma_0(t), \gamma_1(t), \ldots, \gamma_M(t)] \\
\gamma_1(t) &= f_1[t, \gamma_0(t), \gamma_1(t), \ldots, \gamma_M(t)] \\
&\vdots \\
\gamma_M(t) &= f_M[t, \gamma_0(t), \gamma_1(t), \ldots, \gamma_M(t)]
\end{align*}
\]  

(5.4)

and also in a matrix-vector form as

\[
\frac{d\gamma(t)}{dt} = \mathbf{A}(t)\gamma(t) + \mathbf{f}(t)\mathbf{1}.
\]  

(5.5)

5.1. Master equations

In the case of the master equations, the coefficient matrix \(\mathbf{A}\) is time-independent, so Eq. (5.5) has a simple solution [51]

\[
\gamma(t) = e^{\mathbf{A}t}\gamma(0),
\]  

(5.6)

where \(\gamma(0)\) is a vector consisting of the initial values. In the case of the eigenstate master equation, we already have analytical solution for the off-diagonal elements in Eq. (4.60). It therefore remains to solve the time evolution of the diagonal elements. They can be written as a column vector

\[
\hat{\rho}(t) = \begin{pmatrix} \rho_{00}(t) \\ \rho_{11}(t) \\ \vdots \\ \rho_{MM}(t) \end{pmatrix}.
\]  

(5.7)
The coefficient matrix consists of the transitions rates:

$$\Lambda = \left( \begin{array}{cccc}
\Gamma_{0 \rightarrow 0} & \Gamma_{0 \rightarrow 1} & \cdots & \Gamma_{0 \rightarrow M} \\
\Gamma_{1 \rightarrow 0} & -\sum_{\beta \neq 1} \Gamma_{1 \rightarrow \beta} & \cdots & \Gamma_{1 \rightarrow M} \\
\vdots & \vdots & \ddots & \vdots \\
\Gamma_{M \rightarrow 0} & \Gamma_{M \rightarrow 1} & \cdots & -\sum_{\beta \neq M} \Gamma_{M \rightarrow \beta}
\end{array} \right). \quad (5.8)
$$

Thus, we obtain the time evolution of the density operator diagonal elements by applying Eq. (5.6):

$$\tilde{\rho}(t) = e^{\Lambda t} \tilde{\rho}(0). \quad (5.9)
$$

The same can also be done for the quantum optical master equation, but here the diagonal elements depend on the off-diagonal elements and vice versa. Consequently, the matrix $\Lambda$ is more complicated and larger and, therefore, the matrix exponential is a bit slower to calculate than with the eigenstate master equation. Note that if one solves the quantum optical master equation using Eqs. (4.46) - (4.49), the resulting density operator is represented in the product basis $\{|i, n\}$ instead of the Hamiltonian eigenbasis $\{|k\}$. The occupation probabilities of the Hamiltonian eigenstates using quantum optical master equation can be obtained as

$$p_k(t) = \text{Tr} \left[ |k\rangle \langle k| \tilde{\rho}_S(t) \right]. \quad (5.10)
$$

The exponential of a matrix $\Lambda$ can be calculated by using the Taylor series:

$$e^{\Lambda t} = \sum_{n=0}^{\infty} \frac{\Lambda^n t^n}{n!}. \quad (5.11)
$$

However, this is not very efficient. If one can calculate the eigenvalues $\lambda_0, \ldots, \lambda_M$ of the matrix $\Lambda$, one can use the Lagrange interpolation method [51], defined as

$$e^{\Lambda t} = \sum_{j=0}^{M} e^{\lambda_j t} \prod_{k \neq j}^{M} \frac{\Lambda - \lambda_k I}{\lambda_j - \lambda_k}. \quad (5.12)
$$

This works only if all the eigenvalues have different values, which is the case for our set of differential equations. The eigenstate master equation was solved with this algorithm. For the quantum optical master equation this was not the most efficient method. It was thus solved with the traditional fourth order Runge–Kutta algorithm, which can be written for the set of differential equations (5.5) [52, 53] as

$$\vec{y}(t_{i+1}) = \vec{y}(t_i) + \tilde{k}_1 + \frac{\tilde{k}_2}{2} + \frac{\tilde{k}_3}{2} + \frac{\tilde{k}_4}{6}, \quad (5.13)
$$

where

$$\tilde{k}_1 = h\vec{f}[t_i, \vec{y}(t_i)], \quad (5.14)
$$

$$\tilde{k}_2 = h\vec{f}[t_{i+1/2}, \vec{y}(t_i) + \tilde{k}_1/2], \quad (5.15)
$$

$$\tilde{k}_3 = h\vec{f}[t_{i+1/2}, \vec{y}(t_i) + \tilde{k}_2/2], \quad (5.16)
$$

$$\tilde{k}_4 = h\vec{f}[t_{i+1}, \vec{y}(t_i) + \tilde{k}_3]. \quad (5.17)
$$

In order to obtain the value of the vector $\vec{y}$ at time $t_i$, one has to know its value at time $t_{i-1}$.

### 5.2. Stochastic Liouville–von Neumann equation

Before describing the algorithm for solving the stochastic Liouville–von Neumann equation, let us discuss the numerical creation of the complex noise terms in Eqs. (4.138) - (4.142). We first have to express our continuous functions in time interval $] - \infty, \infty[$ on a discrete and finite grid $] - t_{N/2}, t_{N/2}[$, where $N$ is the number of points in the grid. We set the time step $h$ to be constant, so that an individual grid point can be written as $t_l = lh$ with $l = 0, \pm 1, \pm 2, \ldots$. Thus, our integrals can be represented as sums and continuous Fourier transforms as discrete Fourier transforms in the frequency grid $\omega_k = 2\pi k/(Nh)$, where $k = 0, \pm 1, \ldots, \pm N/2$ [10]. We use the Cooley–Tukey algorithm to numerically calculate the fast Fourier transforms (FFT), which requires that the
number of points $N$ in the grid is some integer power of 2, i.e. $N = 2^n$ where $n$ is a positive integer. The Fourier transform (4.102) and the inverse Fourier transform (4.104) of the correlation function $L(t)$ can now be written as

$$
\hat{L}(\omega_k) = \frac{1}{N} \sum_{i=0}^{N-1} L(t_i) e^{-2\pi i \omega_k / N}, \quad (5.18)
$$

$$
L(t_i) = \frac{1}{N} \sum_{k=0}^{N-1} \hat{L}(\omega_k) e^{2\pi i \omega_k / N}. \quad (5.19)
$$

Here the sign of the Fourier exponent has been changed to that used in the numerical algorithms [10]. Similarly, the integral in Eq. (4.138) can be discretized as

$$
\tilde{\zeta}_R(t_j) = \frac{1}{N} \sum_{i=0}^{N-1} G(t_{j-i}) x(t_i), \quad (5.20)
$$

and the rest of the Eqs. (4.139) - (4.142) similarly. Gaussian white noise (4.98) is now

$$
\langle x(t_j) x(t_i) \rangle = \delta_{ij}, \quad (5.21)
$$

i.e. the Dirac delta function is changed into a Kroenecker delta.

Let us then present the algorithm for calculating the noises. We use the $\zeta_R$ noise as an example, but the same procedure applies also to the rest of the noise terms. We start by choosing a suitable maximum time $t_{N/2}$ and the number of data points $N$. The time step is then $h = 2t_{N/2}/N$. We then produce a time array of the form

$$
[t_0, t_1, t_2, \ldots, t_{N/2}, -t_{N/2}, \ldots, -t_2, -t_1],
$$

i.e. first half of the array consists of positive times and the remaining half contains the negative times. This is the form most numerical libraries handle the Fourier transforms. We set $t_0 = 0$. Next, we integrate numerically Eq. (3.72) to obtain $L(t_i)$. In the case of $\zeta_R$, we then take the discrete Fourier transform of $L_R(t_i)$ and obtain

$$
\hat{L}_R(\omega_k) = \frac{1}{N} \sum_{i=0}^{N-1} L_R(t_i) e^{-2\pi i \omega_k / N}. \quad (5.22)
$$

We then obtain the window function by taking the square root

$$
\hat{G}(\omega_k) = \sqrt{\hat{L}_R(\omega_k)}. \quad (5.23)
$$

In the case of Ohmic spectral density with the Drude cutoff (3.81), we were able to calculate analytic forms for the window functions $\hat{G}(\omega)$ and $\hat{W}(\omega)$ (Eqs. (4.143) and (4.144)). Thus, we can produce an array consisting of the frequencies:

$$
[\omega_0, \omega_1, \ldots, \omega_{N/2}, -\omega_{N/2}, \ldots, -\omega_2, -\omega_1], \quad \omega_k = k2\pi/(Nh),
$$

and calculate directly $\hat{G}(\omega_k)$ and $\hat{W}(\omega_k)$, without a need to solve $L(t_i)$.

Next, we create an array consisting of the random Gaussian variables $x(t_i)$ and take the discrete Fourier transform

$$
\hat{x}(\omega_k) = \frac{1}{N} \sum_{i=0}^{N-1} x(t_i) e^{-2\pi i \omega_k / N} \quad (5.24)
$$

and then take the inverse Fourier transform of $\hat{G}(\omega_k) \hat{x}(\omega_k)$ to obtain $\zeta_R(t_j)$:

$$
\zeta_R(t_j) = \frac{1}{N} \sum_{i=0}^{N-1} G(t_{j-i}) x(t_i) = \frac{1}{N^2 h^2} \sum_{i=0}^{N-1} \sum_{k=0}^{N-1} \sum_{n=0}^{N-1} \hat{G}(\omega_k) \hat{x}(\omega_k) e^{2\pi i (j-i) / N} e^{2\pi i n k / N} \quad (5.25)
$$

$$
= \frac{1}{Nh} \sum_{k=0}^{N-1} \hat{G}(\omega_k) \hat{x}(\omega_k) e^{2\pi i k j / N}, \quad (5.26)
$$

where we have used the relation

$$
\sum_{l=0}^{N-1} e^{2\pi i (n-k)/N} = N \delta_{nk}. \quad (5.27)
$$
Notice that in Eq. (5.22) \( L_R(\omega_k) \) is proportional to the time step \( h \), and this holds also for \( L_I(\omega_k) \). When we calculate the window functions, we take the square root, so our window functions \( \tilde{G}(\omega_k) \) and \( \tilde{W}(\omega_k) \), and therefore also our noises \( \xi(t_j) \) and \( \nu(t_j) \), are actually proportional to the square root of the time step. To eliminate this, we have to divide the noise in Eq. (5.26) by \( \sqrt{h} \). Note also that because we have defined the discrete Fourier transforms with the opposite sign in the exponent, we have to swap the window function \( \tilde{W}(\omega_k) \) with its complex conjugate in the definitions of the complex \( \zeta \) and \( \nu \) noises. After doing these, we can write Eqs. (4.138) - (4.142) as

\[
\begin{align*}
\xi_R(t_j) &= \frac{1}{N\sqrt{h}} \sum_{k=0}^{N-1} \tilde{G}(\omega_k) \tilde{z}(\omega_k) e^{i2\pi kj/N}, \\
\xi_C(t_j) &= \frac{1}{N\sqrt{h}} \sum_{k=0}^{N-1} W^*(\omega_k) \hat{z}_1(\omega_k) e^{i2\pi kj/N}, \\
\xi_p(t_j) &= \frac{1}{N\sqrt{h}} \sum_{k=0}^{N-1} W^*(\omega_k) \hat{z}_2(\omega_k) e^{i2\pi kj/N}, \\
\nu_R(t_j) &= -\frac{1}{N\sqrt{h}} \sum_{k=0}^{N-1} \tilde{W}(\omega_k) \hat{z}_2(\omega_k) e^{i2\pi kj/N}, \\
\nu_C(t_j) &= -\frac{1}{N\sqrt{h}} \sum_{k=0}^{N-1} \tilde{W}(\omega_k) \hat{z}_1(\omega_k) e^{i2\pi kj/N},
\end{align*}
\]

where the window function \( \tilde{W}(\omega_k) \) is

\[
\tilde{W}(\omega_k) = \left\{ \frac{1}{2} \left[ \tilde{X}(\omega_k) - \mu \right] \right\}^{1/2}.
\]

Now that we have the noises defined on the time interval \([t_0, t_1, \ldots, t_{N/2}, \ldots, -t_1]\), we can proceed to solve \( \rho_S(t) \) on the positive time interval, i.e. \([t_0 = 0, \ldots, t_{N/2} = 2]\). We present here the trapezoidal method we use in our computations. We first write the density operator matrix elements as a column vector:

\[
\bar{\rho}(t) = \begin{pmatrix} \rho_{00}(t) & \rho_{01}(t) & \cdots & \rho_{0M}(t) & \rho_{1M}(t) \end{pmatrix}^T
\]

Thus, our set of differential equations can be written as

\[
\frac{d\bar{\rho}(t)}{dt} = \tilde{f}[t, \bar{\rho}(t)]
\]

with some initial value \( \bar{\rho}(0) \). We first integrate Eq. (5.35) from \( t_i \) to \( t_{i+1} \):

\[
\bar{\rho}(t_{i+1}) = \bar{\rho}(t_i) + h \int_{t_i}^{t_{i+1}} \tilde{f}[t, \bar{\rho}(t)] dt \approx \bar{\rho}(t_i) + \frac{h}{2} \left[ \tilde{f}[t_i, \bar{\rho}(t_i)] + \tilde{f}[t_{i+1}, \bar{\rho}(t_{i+1})] \right].
\]

Note that we have \( \bar{\rho}(t_{i+1}) \) on both sides of the equation, and, thus, we have to solve \( \bar{\rho}(t_{i+1}) \) iteratively. An initial guess is obtained from the Euler method for the differential equations [10, 53]:

\[
\bar{\rho}(t_{i+1}) = \bar{\rho}(t_i) + h\tilde{f}[t_i, \bar{\rho}(t_i)].
\]

Thus, if we know \( \bar{\rho}(t_i) \), we can calculate \( \bar{\rho}(t_{i+1}) \).

The algorithm for solving the stochastic Liouville–von Neumann equation can be written as follows:

1) Calculate the window functions.
2) Generate three Gaussian noises and take their Fourier transforms.
3) Calculate the noises \( \xi(t) \) and \( \nu(t) \).
4) Solve the stochastic Liouville–von Neumann equation and store calculated \( \bar{\rho}(t) \)
5) Go back to 2) sufficiently many times, i.e. calculate different samples.
6) Take the average of all stored \( \bar{\rho}(t) \)'s to obtain the system density operator \( \rho_S(t) \). (Individual samples have no physical meaning, but their average converges towards the physical density operator.)

We have solved the stochastic Liouville–von Neumann equation in the product basis \( \{|n\} \). The transformation to the Hamiltonian eigenbasis is the same as with the quantum optical master equation (Eq. (5.10)).
5.3. Code

Both master equations and the stochastic Liouville–von Neumann equation were solved with Fortran95. Eigen-problems were solved with the LAPACK [54] routines and some matrix multiplication was enhanced with the BLAS [55]. Fourier transforms were performed with the FFTW [56] library (Fastest Fourier Transforms in the West). Python 3.5 from the Anaconda distribution [57] was used for scripting and parallelizing the computation. Some numerical calculation was done also with Python using NumPy and SciPy libraries [58]. Most of the analytical results were checked with SymPy [59]. All plots were produced with Python’s Matplotlib library [60].

5.4. Initial values and parameters

We have two sets of basis states that we can choose as our initial states: the Hamiltonian eigenbasis and the product basis, which is also the eigenbasis of the uncoupled Hamiltonian ($g = 0$). We will see that although the steady state does not depend on the initial state [41], the time evolution in some cases does. We used two different initial states: the ground state $|0\rangle$ of the Hamiltonians (3.11) and (3.21) and the first excited product state $|\uparrow 0\rangle$. If we transform $|\uparrow 0\rangle$ into the Hamiltonian eigenbasis, we see that some of the off-diagonal elements of the reduced density operator are initially non-zero. This causes some peculiarities in the time evolution (Recall that in the eigenstate master equation the diagonal elements are decoupled from the off-diagonal elements of the density operator, whereas in the quantum optical master equation they are not).

The time evolution given by the master equations describes exponential decay. In reality this is only approximately true, and with the stochastic Liouville–von Neumann equation we should see initial evolution that deviates from pure exponential decay. We expect that with decreasing environmental coupling this difference becomes smaller.

In the numerical simulations we have set the natural constants $\hbar$ and $k_B$ to unity. We have set the unit of angular frequency to be $\omega_c$, thus the unit of time is $2\pi/\omega_c$. We have studied three different cases: resonance of the qubit and the cavity, $\omega_c = \omega_0$, and two detuned regimes: $\omega_c > \omega_0$ and $\omega_c < \omega_0$. We study how the strength of the coupling $g$ affects the time-evolution and the steady state of our equations. We also study the effect of $\eta$, i.e. the strength of the environmental coupling. Thus, we compare the solutions of the three equations with different values of $g$ and $\eta$, and study the effects of the relative strengths of $\omega_c$, $g$ and $\eta$.

In the larger the temperature, the more stable the solution to the stochastic Liouville–von Neumann equation is, i.e. it requires less samples to reach convergent solutions. We were able to produce convergent solutions with $T = 1$, but only in resonance. The Drude cutoff frequency $\omega_D$ also affects the stability of the solutions of the stochastic Liouville–von Neumann equation, and it also affects the time step size in the integration: $\hbar$ must be much smaller than $1/\omega_D$. Thus, we have chosen $\omega_D = 5$. The coefficient $q_0$ is kept equal to unity, since its effect is just similar to that of $\eta$.

The size of the system also affects the stability of the stochastic Liouville–von Neumann equation. The more basis states one takes, the less stable the solutions become, and consequently the computation time is longer. But, since the temperature is low, we do not need many basis states. We have found the solutions for the stochastic Liouville–von Neumann equation with three and four states in the cavity, i.e. the Hamiltonian has six or eight basis states, respectively. For the master equations, the number of the basis states is not a problem: our program can easily handle systems where the cavity has 50 basis states, but for our temperature values it is not necessary to go that far. Increasing the cavity eigenstates beyond three or four changes the results only negligibly with our parameter values.
6. Results

6.1. Uncoupled qubit and cavity

Let us first consider a situation in which the qubit and the cavity are decoupled (Figure 4). The solutions of the quantum optical (QO) master equation and the eigenstate (ES) master equation are identical, and the steady state is exactly described by the Gibbs distribution. The stochastic Liouville–von Neumann (SLN) equation has small deviations from the solutions of the master equations. Because the coupling is zero, the initial state of the qubit remains unchanged throughout the evolution. The trace of the density operator is also plotted. For the master equations it is unity at all times. The trace of the density operator calculated from the stochastic Liouville–von Neumann equation approaches unity with sufficient number of samples. From the following figures one can observe that even though the trace given by the stochastic Liouville–von Neumann equation is unity at short simulation times, it begins to deviate from that after sufficient amount of time has passed. This happens because the simulation reaches the critical time, after which the solutions of the stochastic Liouville–von Neumann equation are no longer stable.

![Figure 4: Time evolution of the diagonal elements of the density matrix of the uncoupled system. Solid lines give the solution of the stochastic Liouville–von Neumann equation, the dashed lines that of the eigenstate master equation and the dotted lines that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|0\rangle$. Parameters are: $\eta = 0.05408$, $\kappa = 0.1$, $T = 1$, $\omega_D = 5$, $\omega_c = 1$ and $\omega_0 = 1$. Number of system eigenstates used for the computation: 6. Number of data points: $2^{14}$. Total number of samples: 150000 (divided equally between three processor cores). Total computation time of the SLN equation: 6050s.](image)

6.2. Resonance

Let us then consider a finite coupling between the qubit and the cavity in resonance. From now on, we will use the Rabi Hamiltonian.
6.2.1. Weak qubit-cavity coupling

Let us first consider a situation where the coupling between the qubit and the cavity is weak \((g = 0.01)\). The situation where all three equations agree well with each other \((\kappa < g \ll \omega)\) is shown in Figure 5. Figure 5a shows the evolution starting from the initial state \(\ket{0}\). All equations produce nearly the same evolution, but the stochastic Liouville–von Neumann equation becomes numerically unstable before reaching the steady state. In the Figure 5b the system was initially in the thermal state given by the Gibbs distribution. This is the steady state of the eigenstate master equation, but also the quantum optical master equation and the stochastic Liouville–von Neumann equation demonstrate very similar behaviour.

We can then increase the environmental coupling to be of the same order of magnitude as the qubit-cavity coupling, \((\kappa \sim g \ll \omega)\). This situation is shown in Figure 6. From Figure 6a we observe that the evolution produced by the eigenstate master equation no longer agrees with the stochastic Liouville–von Neumann equation. The solution of the quantum optical master equation, on the other hand, fits quite well with the stochastic Liouville–von Neumann equation. As we discussed earlier, the secular approximation we made in the derivation of the eigenstate master equation is valid only if the qubit-cavity coupling is much larger than the environmental coupling, which is not the case here. The steady states of the stochastic Liouville–von Neumann equation and the quantum optical master equation, however, still agree well with the steady state of the eigenstate master equation, as shown in Figure 6b.

If we increase the environmental coupling even more, the solution of the eigenstate master equation differs even more from the stochastic Liouville–von Neumann equation, but also the differences between the solutions of the quantum optical master equation and the stochastic Liouville–von Neumann equation start to increase, as shown in Figure 7. The time evolution of the stochastic Liouville–von Neumann equation and the quantum optical master equation is now much slower than that of the eigenstate master equation (Figure 7a). The steady state solution of the stochastic Liouville–von Neumann equation also begins to differ notably from the Gibbs distribution (Figure 7b) in such way that the steady state occupation probability of the ground state is a bit smaller and the occupation probabilities of the excited states a bit larger than given by the Gibbs distribution. This can be interpreted as a thermal distribution in a higher temperature (or a Lamb shift of the energy levels). In the stochastic Liouville–von Neumann equation the system thus effectively ‘feels’ a larger temperature than in the master equations.

By increasing the environmental coupling to be of the same order as the uncoupled system energies, all three equations produce completely different results as shown in Figure 8. This parameter region is clearly beyond the validity of the master equations since the environmental coupling can no longer be treated as a perturbation, thus breaking the Born approximation. The solutions of the stochastic Liouville–von Neumann equation are no longer nearly exponential.
Figure 5: Time evolution of the diagonal elements of the density matrix of the system with weak qubit-cavity coupling and even weaker environmental coupling. Solid lines give the solution of the stochastic Liouville–von Neumann equation, dashed lines that of the eigenstate master equation and dotted lines that of the quantum optical master equation. Initial state was determined by a) the state $|0\rangle$; b) the Gibbs distribution. System was described by the Rabi Hamiltonian. Parameters are: $\eta = 0.0005408$, $\kappa = 0.001$, $T = 1$, $\omega_0 = 5$, $\omega_c = 1$, $\omega_b = 1$ and $g = 0.01$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{19}$. Total number of samples: 40000 (divided equally between three processor cores). Total computation time of the SLN equation: 79000s.

Figure 6: Time evolution of the diagonal elements of the density matrix of the system with weak qubit-cavity coupling. The environmental coupling is equal to the qubit-cavity coupling ($\kappa = g$). Initial state was determined by a) the state $|0\rangle$; b) Gibbs distribution. System was described by the Rabi Hamiltonian. Parameters are: $\eta = 0.0005408$, $\kappa = 0.01$, $T = 1$, $\omega_0 = 5$, $\omega_c = 1$, $\omega_b = 1$ and $g = 0.01$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{18}$. Total number of samples: 30000 (divided equally between three processor cores). Total computation time of the SLN equation: 20000s.
Figure 7: Time evolution of the diagonal elements of the density matrix of the system with weak qubit-cavity coupling and medium environmental coupling. Initial state was determined by a) the state $|0\rangle$; b) Gibbs distribution. System was described by the Rabi Hamiltonian.
Parameters are: $\eta = 0.05408$, $\kappa = 0.1$, $T = 1$, $\omega_D = 5$, $\omega_c = 1$, $\omega_0 = 1$ and $g = 0.01$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{14}$. Total number of samples: 300000 (divided equally between three processor cores). Total computation time of the SLN equation: 12000s.

Figure 8: Time evolution of the diagonal elements of the density matrix of the system with weak qubit-cavity coupling and strong environmental coupling. Initial state was determined by the state $|0\rangle$.
Parameters are: $\eta = 0.5408$, $\kappa = 1$, $T = 1$, $\omega_D = 5$, $\omega_c = 1$, $\omega_0 = 1$ and $g = 0.01$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{10}$. Total number of samples: 1500000 (divided equally between three processor cores). Total computation time of the SLN equation: 3400s.
6.2.2. Medium qubit-cavity coupling

Let us then increase the coupling between the qubit and the cavity \((g = 0.1)\) and repeat the steps in the weak coupling discussion. The assumption that the qubit and the cavity are decoupled is clearly not valid and therefore the quantum optical master equation itself is no longer valid. We begin with the weak environmental coupling, shown in Figure 9. One can see that, as expected, the solution of the quantum optical master equation differs significantly from that of the eigenstate master equation. This is the most visible from the evolution of the occupation probabilities of the two lowest excited states \(|1\rangle\) and \(|2\rangle\), which, according to the quantum optical master equation, evolve very closely together. The solution of the eigenstate master equation, however, shows them evolving further away from each other. This same phenomena is also observed for the higher excited states, but those are not shown here. The evolution produced by the stochastic Liouville–von Neumann equation agrees extremely well with the eigenstate master equation. From Figure 9b, one can see that the steady state of the stochastic Liouville–von Neumann equation is very close to the Gibbs distribution. The steady state of the quantum optical master equation, on the other hand, is not.

If we increase the environmental coupling to be equal to the qubit-cavity coupling, we see in Figure 10 that also the eigenstate master equation starts to deviate from the stochastic Liouville–von Neumann equation, as expected. The time evolution of the occupation probabilities of the states calculated from the master equations no longer agrees with the stochastic Liouville–von Neumann equation, which can be seen from Figure 10a. The steady state of the stochastic Liouville–von Neumann equation also starts to deviate from the Gibbs distribution, but it is still much closer to that than the solution of the quantum optical master equation (Figure 10b).

By increasing the environmental coupling even further, we again observe clear differences between the solutions of the three equations (Figure 11).

![Figure 9](image)

**Figure 9:** Time evolution of the diagonal elements of the density matrix of the system with medium qubit-cavity coupling and weak environmental coupling. Solid line is the solution of the stochastic Liouville–von Neumann equation, dashed line that of the eigenstate master equation and dotted line that of the quantum optical master equation. Initial state was determined by a) the state \(|0\rangle\); b) Gibbs distribution. System was described by the Rabi Hamiltonian. Parameters are: \(\eta = 0.005408\), \(\kappa = 0.01\), \(T = 1\), \(\omega_0 = 5\), \(\omega_k = 1\), \(\omega_0 = 1\) and \(g = 0.1\). Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: \(2^{18}\). Total number of samples: 60000 (divided equally between three processor cores). Total computation time of the SLN equation: 39000s.
Figure 10: Time evolution of the diagonal elements of the density matrix of the system with medium qubit-cavity coupling and medium environmental coupling. Initial state was determined by a) the state $|0\rangle$; b) Gibbs distribution.
Parameters are: $\eta = 0.05408$, $\kappa = 0.1$, $T = 1$, $\omega_0 = 5$, $\omega_k = 1$, $\omega_0 = 1$ and $g = 0.1$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{14}$. Total number of samples: 300000 (divided equally between three processor cores). Total computation time of the SLN equation: 11000s.

Figure 11: Time evolution of the diagonal elements of the density matrix of the system with medium qubit-cavity coupling and strong environmental coupling. Initial state was determined by the state $|0\rangle$.
Parameters are: $\eta = 0.5408$, $\kappa = 1$, $T = 1$, $\omega_0 = 5$, $\omega_k = 1$, $\omega_0 = 1$ and $g = 0.01$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{10}$. Total number of samples: 1500000 (divided equally between three processor cores). Total computation time of the SLN equation: 3800s.
6.2.3. Strong qubit-cavity coupling

Let us then set the qubit-cavity coupling to be equal to the energies of the qubit and the cavity. Starting again from the weak environmental coupling we see from Figure 12 that the solutions of the stochastic Liouville–von Neumann equation and the eigenstate master equation agree extremely well. The solution of the quantum optical master equation, as expected, is totally different. The steady state of the stochastic Liouville–von Neumann equation is very close to the Gibbs distribution. The steady state of the quantum optical master equation, however, is way off. By increasing the environmental coupling the solutions of the stochastic Liouville–von Neumann equation and the eigenstate master equation start to deviate, and the steady state of the stochastic Liouville–von Neumann equation is clearly different from the Gibbs distribution, as shown in Figure 13. Difference can again be interpreted by the larger effective temperature experienced by the system. If we then increase the environmental coupling strength to be of the same order as that of the qubit-cavity coupling (now $\kappa = g = \omega$), all three equations give different solutions, as shown in Figure 14.

![Figure 12: Time evolution of the diagonal elements of the density matrix of the system with strong qubit-cavity coupling and weak environmental coupling. Solid line is the solution of the stochastic Liouville–von Neumann equation, dashed line that of the eigenstate master equation and dotted line that of the quantum optical master equation. Initial state was determined by a) the state $|0\rangle$; b) Gibbs distribution. System was described by the Rabi Hamiltonian. Parameters are: $\eta = 0.005408$, $\kappa = 0.01$, $T = 1$, $\omega_D = 5$, $\omega_c = 1$, $\omega_0 = 1$ and $g = 1$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{18}$. Total number of samples: 60000 (divided equally between three processor cores). Total computation time of the SLN equation: 36000s.](image)
Figure 13: Time evolution of the diagonal elements of the density matrix of the system with strong qubit-cavity coupling and medium environmental coupling. Initial state was determined by a) the state $|0\rangle$; b) Gibbs distribution. Parameters are: $\eta = 0.05408$, $\kappa = 0.1$, $T = 1$, $\omega_\phi = 5$, $\omega_\xi = 1$, $\omega_0 = 1$ and $g = 1$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{14}$. Total number of samples: 90000 (divided equally between three processor cores). Total computation time of the SLN equation: 3600s.

Figure 14: Time evolution of the diagonal elements of the density matrix of the system with strong qubit-cavity coupling and strong environmental coupling. Initial state was determined by the state $|0\rangle$. Parameters are: $\eta = 0.5408$, $\kappa = 1$, $T = 1$, $\omega_\phi = 5$, $\omega_\xi = 1$, $\omega_0 = 1$ and $g = 1$. Number of system eigenstates used for the computation: 8 (4 of them are plotted). Number of data points: $2^{10}$. Total number of samples: 1200000 (divided equally between six processor cores). Total computation time of the SLN equation: 2400s.
6.2.4. Changing the initial state

Until now we have only considered cases where the initial state has been the lowest eigenstate $|0\rangle$ of the Hamiltonian (3.11). The above discussion also holds for any other Hamiltonian eigenstate $|n\rangle$. Let us now consider situations where the initial state is one of the product states $|j n\rangle$. This means that in the Hamiltonian eigenbasis the initial density matrix has non-zero elements also in the off-diagonals. Because in the eigenstate master equation the diagonal density matrix elements are independent of the off-diagonals, which decay exponentially, this change of the initial state has no effect on the solutions of the eigenstate master equation.

Let us first consider weak qubit-cavity coupling and a bit weaker environmental coupling, shown in Figure 15. The solution of the eigenstate master equation is again an exponential curve, as expected. The solutions of the stochastic Liouville–von Neumann equation and the quantum optical master equation, on the other hand, display Rabi oscillations [11] around the solutions of the eigenstate master equation. These oscillations then decay while approaching the steady state. The oscillations are caused by the coupling between the diagonal elements and the initially non-zero off-diagonal elements, which is neglected in the secular approximation made in the derivation of the eigenstate master equation.

If we then increase both the qubit-cavity and environmental couplings, we see in Figure 16 that the oscillations in the solutions of the stochastic Liouville–von Neumann equation and the quantum optical master equation start to differ. The quantum optical master equation is no longer valid because of the large qubit-cavity coupling. The solution of the stochastic Liouville–von Neumann equation, on the other hand, agrees quite well with the eigenstate master equation, if the oscillations are neglected.

If we then decrease the qubit-cavity coupling, we observe increase in the oscillation amplitude and decrease in the oscillation frequency, as shown in Figures 17 and 18. Increasing the coupling on the other hand results in the decrease of the oscillation amplitude (Figure 19). The amplitudes of these oscillations seem to be proportional to the ratio $\kappa/g$, as suggested in Ref [11]. Figure 19 further shows that the overall evolutions produced by the stochastic Liouville–von Neumann equation and the eigenstate master equation agree well with each other, although the solutions of the stochastic Liouville–von Neumann equation contain Rabi oscillations.
Figure 15: Time evolution of the diagonal elements of the density matrix of the system with weak qubit-cavity coupling and weak environmental coupling. Solid line is the solution of the stochastic Liouville–von Neumann equation, dashed line that of the eigenstate master equation and dotted line that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|\uparrow 0\rangle$. System was described by the Rabi Hamiltonian. Parameters are: $\eta = 0.005408, \kappa = 0.01, T = 1, \omega_D = 5, \omega_c = 1, \omega_0 = 1$ and $g = 0.05$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{18}$. Total number of samples: 60000 (divided equally between six processor cores). Total computation time of the SLN equation: 37000s.
Figure 16: Time evolution of the diagonal elements of the density matrix of the system with strong qubit-cavity coupling and medium environmental coupling. Solid line is the solution of the stochastic Liouville–von Neumann equation, dashed line that of the eigenstate master equation and dotted line that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state \( |↑\rangle \). System was described by the Rabi Hamiltonian. Parameters are: \( \eta = 0.05408, \kappa = 0.1, T = 1, \omega_0 = 5, \omega_c = 1, \omega_b = 1 \) and \( g = 0.5 \). Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: \( 2^{14} \). Total number of samples: 150000 (divided equally between six processor cores). Total computation time of the SLN equation: 6000s.
Figure 17: Time evolution of the diagonal elements of the density matrix of the system with medium qubit-cavity coupling and medium environmental coupling. Solid line is the solution of the stochastic Liouville–von Neumann equation, dashed line that of the eigenstate master equation and dotted line that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|\uparrow 0\rangle$. System was described by the Rabi Hamiltonian. Parameters are: $\eta = 0.05408$, $\kappa = 0.1$, $T = 1$, $\omega_D = 5$, $\omega_L = 1$, $\omega_B = 1$ and $g = 0.1$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{14}$. Total number of samples: 90000 (divided equally between six processor cores). Total computation time of the SLN equation: 3600s.
Figure 18: Time evolution of the diagonal elements of the density matrix of the system with weak qubit-cavity coupling and medium environmental coupling. Solid line is the solution of the stochastic Liouville–von Neumann equation, dashed line that of the eigenstate master equation and dotted line that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|\uparrow\rangle$. System was described by the Rabi Hamiltonian.

Parameters are: $\eta = 0.05408$, $\kappa = 0.1$, $T = 1$, $\omega_0 = 5$, $\omega_e = 1$, $\omega_c = 1$ and $g = 0.01$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{14}$. Total number of samples: 90000 (divided equally between six processor cores). Total computation time of the SLN equation: 3600s.
Figure 19: Time evolution of the diagonal elements of the density matrix of the system with strong qubit-cavity coupling and medium environmental coupling. Solid line is the solution of the stochastic Liouville–von Neumann equation, dashed line that of the eigenstate master equation and dotted line that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|\uparrow 0\rangle$. System was described by the Rabi Hamiltonian. Parameters are: $\eta = 0.05408$, $\kappa = 0.1$, $\Gamma = 1$, $\omega_D = 5$, $\omega_c = 1$, $\omega_b = 1$ and $g = 1$. Number of system eigenstates used for the computation: 6 (4 of them are plotted). Number of data points: $2^{14}$. Total number of samples: 90000 (divided equally between six processor cores). Total computation time of the SLN equation: 3600s.

We can thus see that in resonance the numerical results agree well with the expectations. If the qubit-cavity coupling is weak and the environmental coupling is even weaker ($\kappa < g \approx 0.01$), all three equations produce nearly the same dynamics. If the environmental coupling is of the same order or larger than the qubit-cavity coupling but still weak in comparison to the uncoupled energies ($\kappa \approx 0.01$), the quantum optical master equation agrees well with the stochastic Liouville–von Neumann equation, but the eigenstate master equation is no longer correct. Thus, in this case the qubit and the cavity should be treated separately, not as a single entity as in the eigenstate master equation. On the other hand, if the qubit-cavity coupling is stronger ($g \geq 0.1$), the quantum optical master equation fails to produce even approximately accurate results, whereas the eigenstate master equation agrees with the stochastic Liouville–von Neumann equation. If the environmental coupling is large enough ($\kappa = 0.1$), both master equations fail since the Born approximation is no longer valid. The correct time evolution produced by the stochastic Liouville–von Neumann equation can no longer be approximated by an exponential curve. Instead, it seems to initially be parabolic, which transforms to exponential in later times. This is actually true for all solutions of the stochastic Liouville–von Neumann equation, but the weaker the environmental coupling is, the earlier the transformation occurs. Parameters with which the master equations agree with the stochastic Liouville–von Neumann equation are gathered in Table 1.

If the initial state is one of the product states instead of the Hamiltonian eigenstates, the initial density matrix in the Hamiltonian eigenbasis has non-zero elements in the off-diagonals. In the steady state the density operator is diagonal, but the initially non-zero off-diagonal elements are coupled to the diagonal elements, which produces damped oscillations of the diagonal elements in the solutions of the quantum optical master equation and the stochastic Liouville–von Neumann equation. The eigenstate master equation fails to predict these since in it the diagonal elements are independent on the off-diagonals. Apart from these oscillations, the results are the same as with the initial state being one of the Hamiltonian eigenstates.
The values of the qubit-cavity coupling $g$ with which the solutions of the quantum optical master equation are nearly correct are so small that one can use the Jaynes–Cummings Hamiltonian. But since we are dealing with the exact stochastic Liouville–von Neumann equation, it does not seem reasonable to use approximate Hamiltonian.

Note that in the master equations the environmental coupling appears with the average number of quanta in the bath, which is a function of temperature. Therefore also temperature has some effect on the results: it acts as an additional environmental coupling. In a sense increasing the temperature also increases the environmental coupling. Thus, with larger temperatures the master equations start to deviate from the stochastic Liouville–von Neumann equation with smaller values of $\eta$.

Table 1: Results with the resonant qubit-cavity system. Here cells with x show the parameters with which the master equation in question agrees with the SLN, if the environment is in temperature $T = 1$.

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<th>$g = 0.01$</th>
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<td>$\kappa$</td>
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<td>QO</td>
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6.3. Off-resonance

Let us then consider a detuned system ($\omega_0 \neq \omega_c$). Now the time scales of the evolution are much longer than in resonance. This causes problems with the stochastic Liouville–von Neumann equation since it becomes unstable long time before reaching the steady state. We therefore discuss here only the master equations. We now also include the solutions with the Jaynes–Cummings Hamiltonian and compare them with those obtained with the Rabi Hamiltonian.

In the detuned case, the system begins to evolve in time as if there was no coupling between the qubit and the cavity. Only at later times, the coupling starts to affect the evolution. This occurs because the energy transfer between the qubit and the cavity is the most effective in resonance. If the qubit-cavity coupling is weak, the two master equations produce almost exactly the same time evolution for short times. Situation with $\omega_0 < \omega_c$ is shown in Figure 20 and with $\omega_0 > \omega_c$ in Figure 21. In the latter case, the system has already almost reached the Gibbs distribution, which is the steady state of the eigenstate master equation. There is no visible difference between the results for the two Hamiltonians. However, if we let the system evolve longer, we see that the differences between the two master equations and for the two Hamiltonians start to increase. If $\omega_0 < \omega_c$ (Figure 22), the Rabi Hamiltonian reaches the steady state faster. The solutions of the quantum optical master equation with the Jaynes–Cummings and Rabi Hamiltonians are completely different: the solution with the Rabi Hamiltonian is quite close to the Gibbs distribution, even though the time evolution differs from the eigenstate master equation. The solution with the Jaynes–Cummings Hamiltonian on the other hand is nowhere near Gibbs distribution. If $\omega_0 > \omega_c$ (Figure 23), the eigenstate master equation remains in the Gibbs distribution as expected. The quantum optical master equation continues to evolve further, and it actually produces the same steady state as in Figure 22: the steady state of the quantum optical master equation is independent on the value of $\omega_0$. This was also discussed in Section 4.3.
Figure 20: Short time evolution of the system density operator with $\omega_0 < \omega_c$ and weak qubit-cavity coupling. Solid line is the solution of the eigenstate master equation and dashed line that of the quantum optical master equation. The solutions are almost identical. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|0\rangle$. System was described by a) the Jaynes–Cummings Hamiltonian; b) the Rabi Hamiltonian. Parameters are: $\kappa = 0.001$, $T = 1$, $\omega_D = 5$, $\omega_k = 1$, $\omega_0 = 0.1$ and $g = 0.01$. Number of system eigenstates used for the computation: 10 (6 of them are plotted).

Figure 21: Short time evolution of the system density operator with $\omega_0 > \omega_c$ and weak qubit-cavity coupling. System was described by a) the Jaynes–Cummings Hamiltonian; b) the Rabi Hamiltonian. Parameters are: $\kappa = 0.001$, $T = 1$, $\omega_D = 5$, $\omega_k = 1$, $\omega_0 = 11$ and $g = 0.1$. Number of system eigenstates used for the computation: 10.
Let us then increase the qubit-cavity coupling. Now we observe differences between the solutions of the master equations also with earlier times, as shown in Figures 24 and 25 for situations $\omega_0 < \omega_c$ and $\omega_0 > \omega_c$, respectively. From these figures one can again observe that the solutions with the Rabi Hamiltonian evolve faster than the solutions with the Jaynes–Cummings Hamiltonian. The resulting steady states are similar to those shown in Figures 22 and 23 and are thus not shown here.

If we increase the qubit-cavity coupling even further, we observe drastic differences between the two master equations and the two Hamiltonians. From Figure 26 one can observe that the solution of the quantum optical master equation with the Jaynes–Cummings Hamiltonian no longer even slightly resembles that of the eigenstate master equation. In the case of the Rabi Hamiltonian the solutions are a bit more similar.

These numerical simulations show that in off-resonance the quantum optical master equation does not produce a steady state that is even close to the Gibbs distribution (4.149). The steady state of the quantum optical master
equation is independent on the values of $\omega_0$ and $g$, and with the Jaynes–Cummings Hamiltonian it is always described by the distribution given in Eq. (4.158). In off-resonance these are not even close. However, if the qubit-cavity coupling is weak and $\omega_0 > \omega_c$, the solution of the quantum optical master equation stays for a while near the Gibbs distribution. If one stops the simulation there, one can obtain almost correct results. Here one should use the Jaynes–Cummings Hamiltonian, since it seems to stay at the Gibbs distribution longer. On the other hand, if $\omega_0 < \omega_c$, the steady state of the quantum optical master equation with the Rabi Hamiltonian is quite close to the steady state of the eigenstate master equation, even though the evolution is different.

In off-resonance there seems to be no difference between the Hamiltonian eigenstates and product states as initial states: oscillations occur only if the Hamiltonian eigenstates are Bell states or close to them, which happens only near resonance. This is caused by the fact that in off-resonance the Hamiltonian eigenstates are almost the same as the product states.

**Figure 24:** Short time evolution of the system density operator with $\omega_0 < \omega_c$ and medium qubit-cavity coupling. Solid line is the solution of the eigenstate master equation and dashed line that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|0\rangle$. System was described by a) the Jaynes–Cummings Hamiltonian; b) the Rabi Hamiltonian. Parameters are: $\kappa = 0.001$, $T = 1$, $\omega_0 = 5$, $\omega_c = 1$, $\omega_b = 0.1$ and $g = 0.1$. Number of system eigenstates used for the computation: 10 (6 of them are plotted).
**Figure 25:** Short time evolution of the system density operator with $\omega_0 > \omega_c$ and medium qubit-cavity coupling. System was described by a) the Jaynes–Cummings Hamiltonian; b) the Rabi Hamiltonian. Parameters are: $\kappa = 0.001$, $T = 1$, $\omega_D = 5$, $\omega_c = 1$, $\omega_0 = 11$ and $g = 1$. Number of system eigenstates used for the computation: 10.

**Figure 26:** Time evolution of the system density operator with $\omega_0 < \omega_c$ and strong qubit-cavity coupling. Solid line is the solution of the eigenstate master equation and dashed line that of the quantum optical master equation. The Gibbs distribution is described by the black horizontal lines. Initial state was determined by the state $|0\rangle$. System was described by a) the Jaynes–Cummings Hamiltonian; b) the Rabi Hamiltonian. Parameters are: $\kappa = 0.001$, $T = 1$, $\omega_D = 5$, $\omega_c = 1$, $\omega_0 = 0.1$ and $g = 1$. Number of system eigenstates used for the computation: 10 (6 of them are plotted).
7. Conclusions

We have studied the time evolution of a quantum system where a qubit is coupled to a harmonic oscillator describing a cavity. The cavity is further coupled bilinearly to a harmonic oscillator bath. The qubit-cavity system can be described by the Rabi Hamiltonian. If the qubit and the cavity are in resonance and the coupling between them is weak, a rotating wave approximation can be performed, which results in the Jaynes–Cumming Hamiltonian whose eigenvalues and eigenvectors can be solved analytically. The interaction between the system and the environment causes dissipation of energy from the system to the environment, but also absorption from the environment to the system. This dynamical process can be solved in formally exact manner with the path integral formalism. In the case of a bilinearly coupled oscillator bath, the cumbersome path integrals can be written into the form of the stochastic Liouville–von Neumann equation, which gives the reduced density operator of the system as a function of time. If the coupling between the system and the environment is weak, one can make the Born–Markov approximation and obtain a perturbative master equation in Lindblad form. The quantum optical master equation has been successfully used, for example, in quantum optics. However, its derivation assumes that the qubit and the cavity are decoupled, which restricts its use only to the weak coupling limit. The dissipators of the quantum optical master equation induce transitions between the eigenstates of the cavity, not between the eigenstates of the system Hamiltonian. The other master equation we studied, the eigenstate master equation, treats the qubit-cavity system as a single entity and, consequently, the transitions induced by the environment occur between the system eigenstates. However, this equations is only valid if the environmental coupling is much weaker than the qubit-cavity coupling.

We showed that the diagonal elements of the reduced density operator obey the same equations of motion for the two perturbative approaches if there is no coupling between the qubit and the cavity, but the off-diagonal elements do not. According to the eigenstate master equation they evolve independent on each other and decay exponentially. In the quantum optical master equation they depend on each other. This difference is caused by the secular approximation. If the qubit and the cavity are coupled, the two master equations give different equations of motion. In the quantum optical master equation the diagonal elements are now depending also on the off-diagonal elements and vice versa. This does not happen with the eigenstate master equation: the off-diagonal elements are still independent on each other and on the diagonal elements. Eventually, the solutions of both master equations reach a steady state. The steady state of the eigenstate master equation was shown to be exactly the Gibbs distribution. The steady state of the quantum optical master equation with the Jaynes–Cummings Hamiltonian was the Gibbs distribution with the uncoupled resonant Hamiltonian, also in the detuned case, and it is independent on the angular frequency of the qubit and the qubit-cavity coupling.

We numerically studied the solutions of the three equations with different parameters. In resonance, all three equations produce almost the same results if the coupling between the qubit and the cavity is much weaker than the uncoupled energies of the qubit and the cavity, and if the environmental coupling is even weaker. If the environmental coupling is of the same order of magnitude or larger than the qubit-cavity coupling, the solutions of the stochastic Liouville–von Neumann equation and the quantum optical master equation are almost the same, but the eigenstate master equation is no longer valid. The difference is seen only in the time evolution: all three equations produce almost the same steady states. If the environmental coupling is large enough, also the quantum optical master equation fails, since the Born approximation no longer holds. If the qubit-cavity coupling is stronger, the quantum optical master equation fails for all values of the environmental coupling. The eigenstate master equation agrees with the stochastic Liouville–von Neumann equation as long as the environmental coupling is weaker than the qubit-cavity coupling. If the initial state of the system is one of the product states, i.e. the eigenstates of the uncoupled Hamiltonian, the corresponding initial density operator in the Hamiltonian eigenbasis has non-zero elements not only in the diagonal but also in the off-diagonals. This causes Rabi oscillations in the eigenstate occupation probabilities given by the stochastic Liouville–von Neumann equation and the quantum optical master equation. The amplitude of these oscillations is proportional to the ratio between the environmental and qubit-cavity couplings. The oscillations are damped when the system evolves towards the steady state. The solutions of the eigenstate master equation, however, remain unchanged.

For a detuned qubit-cavity system, the time scale of the simulations is much longer than in resonance. As a consequence, we were not able to solve the stochastic Liouville–von Neumann equation, since its solutions become unstable long before the system can reach the steady state. The numerical results for the two master equations show that they do not agree with any parameters we used. But if the frequency of the qubit is much larger than that of the cavity and the qubit-cavity coupling is weak, the solution of the quantum optical master equation stays for a while in the Gibbs distribution. If the simulation is stopped here, one can obtain relatively correct ‘quasi’ steady state results with the quantum optical master equation. On the other hand, if the frequency of the qubit is
smaller than that of the cavity, the steady state of the quantum optical master equation with the Rabi Hamiltonian is quite close to the Gibbs distribution, although the transient dynamics differ notably from the eigenstate master equation.

These results show that in resonance the two master equations can be used as approximations of the exact stochastic Liouville–von Neumann equation in different parameter regions if the environmental coupling is weak. If the qubit-cavity coupling is stronger than the environmental coupling, the system has to be treated as a single system, as the eigenstate master equation does. If the environmental coupling is as strong or stronger, the qubit and the cavity must be considered separately like in the quantum optical master equation. In the latter case one can think of the cavity as a part of the qubit environment. An increase in the environmental coupling leads to a larger difference between the exact solution and the solutions of the master equations. The solutions of the master equations are exponential curves, but the exact solutions display parabolic time dependence in the beginning of the evolution and transform into exponentials later. The steady state of the exact solution starts to differ from the Gibbs distribution. This difference can be interpreted as a larger effective temperature observed by the system. The larger the environmental coupling, the larger is this effective temperature.

The difference in the computation times between the stochastic Liouville–von Neumann equation and the master equations is several orders of magnitude. Our Fortran program solved the master equations in less than a second. The shortest computation time for the stochastic Liouville–von Neumann equation was about an hour and the largest nearly 24 hours, although this increase in computation time produced only small enhancements in the accuracy of the solutions. The problem with the stochastic Liouville–von Neumann equation is also that in the low temperatures the solutions become unstable before reaching the steady state. This is most likely a property of the equation itself, since increasing the data points in the simulation did not have a notable effect. Because the eigenstate master equation is in our case real valued, and the diagonal elements are independent on the off-diagonals, its solution can be found faster than that of the quantum optical master equation. The computational time differences between the Rabi Hamiltonian and the Jaynes–Cummings Hamiltonian are negligible, so there seems to be no reason to use the Jaynes–Cummings, apart from the analytical solutions.

We have showed that it is possible to obtain decent numerical solutions of the stochastic Liouville–von Neumann equation for the resonant qubit-cavity system. In the future we would like to obtain solutions for it also in the detuned case. It would also be interesting to find an analytical form for the steady state of the stochastic Liouville–von Neumann equation. In the case of the eigenstate master equation it would be interesting to obtain an improved version which could produce the Rabi oscillations and which would be valid also for cases where the qubit-cavity coupling and the environmental coupling are of the same order of magnitude.
References


