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Application of a Non-Linear Thermodynamic Master Equation to Three-Level Quantum Systems

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Abstract

Dissipative quantum systems are often described in terms of a quantum master equation, typically of a linear, Lindblad-type of form. Such a master equation can arise from several microscopic models, such as the weak-coupling interaction of radiation with matter and the Caldeira-Leggett model. The resultant density matrix equation enables the investigation of general features of the quantum system, like irreversibility, entropy production, and relaxation to equilibrium. It has the general form of a dynamic equation with both reversible and irreversible terms (generated by energy and entropy, respectively). Recently, a new thermodynamic quantum master equation has been proposed by Prof. Dr. H. C. Öttinger, which provides a useful tool for describing dissipative quantum systems.

The dynamics of a two-level system and of a damped harmonic oscillator, both coupled to one heat bath have already been investigated with such a master equation. However, modelling atoms or molecules with two quantum states is insufficient to properly capture physical non-linear regimes, for example, in quantum optics. To go beyond, it is necessary to model the system of interest with a more rich internal structure. Considering three levels offers a compromise between an appropriate degree of complexity and simplicity. This level of description permits to study many phenomena like coherent population trapping, Autler - Townes splitting, electromagnetically induced transparency (EIT), nonlinear susceptibility or stimulated Raman adiabatic passage. In this contribution, we present results from the application of this new non-linear master equation, to a three-level system (often named qutrit) and a harmonic oscillator, each one coupled to two heat baths, in order to explore non-linear phenomena in open quantum systems.

In this Master's thesis, we have focused on the description of three-level quantum systems through master equations for their density matrix, involving a recently proposed non-linear thermodynamic one. In the first part of this work, we focus on a three-level system interacting with two heat baths, a hot and a cold one. We investigate the rate of heat flow from the hot to the cold bath through the quantum system, and how the steady-state is approached. Additional calculations here refer to the rate of entropy production and the evolution of all elements of the density matrix of the system from an arbitrary initial state to their equilibrium or steady-state value. The results will be compared against those of a linear, Lindblad-type master equation designed so that for a quantum system interacting with only one heat bath, the same final Gibbs steady state is attained.

In the second part of this thesis, we focus on the electromagnetically induced transparency (EIT), a phenomenon typically achievable only in atoms with specific energy structures. For a three level system (to which the present study has focused), for example, EIT requires two dipole allowed transitions (the 1-3 and the 2-3) and one forbidden (the 1-2). The phenomenon is observed when a strong laser (termed the control laser) is tuned to the resonant frequency of the upper two levels. Then, as a weak probe laser is scanned in frequency across the other transition, the medium is observed to exhibit both: a) transparency at what was the maximal absorption in the absence of the coupling field, and b) large dispersion effects at the atomic resonance.

We discuss the Hamiltonian describing the phenomenon and we will present results from two types of master equations: a) an empirically modified Von-Neumann one allowing for decays from each energy state, and b) a typical Lindblad one, with time-dependent operators. In the first case, an analytical solution is possible, which has been confirmed through a direct solution of the full master equation. In the second case, only numerical results can be obtained. We present and compare results from the two master equations for the susceptibility of the system with respect to the probe field, and we will discuss them in light also of available experimental data for this very important phenomenon.

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CHAPTER 1

INTRODUCTION

An open quantum system is a quantum system which is found to be in interaction with an external quantum system, the environment. Such a system can also be viewed as a distinguished part of a larger closed quantum system, the other part being the environment. Lately, there is an upsurge of interest in problems concerning an open quantum system, which is an important concept in many fields such as quantum optics, quantum measurement theory, quantum statistical mechanics, quantum information science, quantum cosmology and semi-classical approximations. Quantum optics provided one of the first testing grounds for the application of the formalism of open quantum systems [4].

Quantum theory introduces a deterministic law, the Schrödinger equation, which governs the dynamics of the probability distributions. This equation describes the evolution of chance, that is the dynamics of ensembles of isolated systems. However, as a probabilistic theory quantum mechanics must also encompass the random occurrence of definite events which are the realizations of the underlying probability distributions. In order to effect the occurrence of chance events a quantum system must be subjected to interactions with its surroundings. Master equations are probably the most prevalent tool used in the study of open quantum systems and the density matrix (or density operator) formalism is quite often the language used in such studies. This formalism describes the statistical distribution of quantum states in a system and allows to treat an ensemble of particles statistically.

The theory of open quantum systems addresses the problems of damping and dephasing in quantum systems by the assertion that all real systems of interest are open systems, surrounded by their environments. The environment is the left-over of what is there if the quantum subsystem one is interested in would be absent. There are many approaches to deal with these systems. Among the most well-known methods are the projection operator techniques by the elimination of the environmental degrees of freedom is regarded as a formal projection [2], [5]. As widely applied are the Lindblad master equations which represent the most general set of equations by which the quantum subsystem can be evolved under Markovian and linearity assumptions [2], [6]. Other popular approaches exploit stochastic dynamics [2], [7], path integral formalism [2], [6] or quantum-classical equations [8]. In the latter approach the quantum subsystem is described quantum mechanically, whereas the environment is governed by classical equations. The validity of standard approaches is usually restricted to high temperatures, where quantum effects are supposed to be small. The popular treatment in terms of Lindblad master equations can even be shown to be inconsistent which is known as the failure of the quantum regression hypothesis [5], [8].

Dissipative quantum systems are often described in terms of a quantum master equation, typically of a linear, Lindblad-type of form [9]. Such a master equation can arise from several microscopic models, such as the weak-coupling interaction of radiation with matter and the Caldeira-Leggett model. The resultant density matrix equation enables the investigation of general features of the quantum system, like irreversibility, entropy production, and relaxation to equilibrium. It has the general form of a dynamic equation with both reversible and irreversible terms (generated by energy and entropy, respectively).

Recently, a new thermodynamic quantum master equation has been proposed by Prof. Dr. H. C. Öttinger, which provides a useful tool for describing dissipative quantum systems [8]. A powerful treatment in terms of quantum-classical equations has been used in which the quantum subsystem and the environment couple irreversibly to each other. The environment is described by an extension of the GENERIC formalism of classical nonequilibrium systems, while the dynamics of the quantum subsystem is described by a quantum master equation [8]. The most striking feature of this master equation is its deep non-linearity improving the relaxation behavior of solutions most visibly for low temperatures. For the case where we have a heat bath environment it has been shown in [5] by H. Grabert that the quantum master equation is used in the present work is the Markovian limit of the exact master equation that resulted from the application of a projection operator technique. The equation has been rediscovered in [10] by extending the classical framework of irreversible thermodynamics [11] to open quantum systems.

The dynamics of a two-level system and of a damped harmonic oscillator, both coupled to one heat, bath have already been investigated with such a master equation [8], [12]. However, modelling atoms or molecules with two quantum states is insufficient to properly capture physical non-linear regimes, for example, in quantum optics. To go beyond, it is necessary to model the system of interest with a more rich internal structure. Considering three levels offers a compromise between an appropriate degree of complexity and simplicity. This level of description permits to study many phenomena like coherent population trapping, Autler - Townes splitting, electromagnetically induced transparency (EIT), non-linear susceptibility or stimulated Raman adiabatic passage.

In this work, we are interested in the application of the non-linear quantum master equation to a three-level system (often named qutrit) and a harmonic oscillator, each one coupled to two heat baths, compared to a Lindblad-type of master equation, constructed in order to relax to the same equilibrium (Gibbs state) as the nonlinear one for the special case where the quantum subsystem is coupled to one heat bath. First, we introduce the Lindblad-type of master equation and which is its form for the two cases where we examine. Subsequently, in the next section, the non-linear quantum master equation is presented and again how is formulated for the two systems. Later on, we present the numerical methods that were applied in order to solve the two master equations. The time integration is achieved with an Adams - Bashforth integration scheme. We have also implemented an independent, non-linear matrix algebra solver for computing the steady-state solution of the density matrix. Finally, we show and discuss our results which obtained from the Lindblad-type of and the non-linear thermodynamic quantum master equations for both systems of interest; the three-level (qutrit) and the harmonic oscillator.

Chapter 2

Quantum Mechanics

In this chapter, we present an overview of quantum mechanics and its fundamental elements. Fist, we make a short introduction, then we explain the wave - particle duality, and afterwards we present the Scrödinger equation, which is fundamental equation of quantum mechanics. Finaly, we introduce the Dirac notation, which we are going to use along this work.

2.1 Introduction

Quantum mechanics is a branch of physics which deals with physical phenomena at microscopic scales, where the action is on the order of the Planck constant, h. It departs from classical mechanics primarily at the quantum realm of atomic and subatomic length scales and also, provides a mathematical description of much of the dual particle-like and wave-like behaviour and interactions of energy and matter.

In advanced topics of quantum mechanics, some of these behaviours are macroscopic and emerge at only extreme (i.e., very low or very high) energies or temperatures. The name quantum mechanics derives from the observation that some physical quantities can change only in discrete amounts (quanta), and not in a continuous (analog) way. For example, the angular momentum of an electron bound to an atom or molecule is quantized. In the context of quantum mechanics, the wave particle duality of energy and matter and the uncertainty principle provide a unified view of the behaviour of photons, electrons, and other atomic-scale objects.

The mathematical formulations of quantum mechanics are abstract. A mathematical function known as the wavefunction provides information about the probability amplitude of position, momentum, and other physical properties of a particle. Mathematical manipulations of the wavefunction usually involve the bra - ket notation, also known as Dirac notation, which requires an understanding of complex numbers and linear functionals. The wavefunction treats the object as a quantum harmonic oscillator, and the mathematics is akin to that describing acoustic resonance. Many of the results of quantum mechanics are not easily visualized in terms of classical mechanics. For instance, the ground state in a quantum mechanical model is a non-zero energy state that is the lowest permitted energy state of a system, as opposed to a more ”traditional” system that is thought of as simply being at rest, with zero kinetic energy.

The earliest versions of quantum mechanics were formulated in the first decade of the 20th century. At around the same time, the atomic theory and the corpuscular theory of light (as updated by Einstein) first came to be widely accepted as scientific fact; these latter theories can be viewed as quantum theories of matter and electromagnetic radiation, respectively. Early quantum theory was significantly reformulated in the mid - 1920s by Werner Heisenberg, Max Born and Pascual Jordan, who created matrix mechanics; Louis de Broglie and Erwin Schrdinger (Wave Mechanics); and Wolfgang Pauli and Satyendra Nath Bose (statistics of subatomic particles). And the Copenhagen interpretation of Niels Bohr became widely accepted. By 1930, quantum mechanics had been further unified and formalized by the work of David Hilbert, Paul Dirac and John von Neumann, with a greater emphasis placed on measurement in quantum mechanics, the statistical nature of our knowledge of reality, and philosophical speculation about the role of the observer. Quantum mechanics has since branched out into almost every aspect of 20th century physics and other disciplines, such as quantum chemistry, quantum electronics, quantum optics, and quantum information science. Much 19th century physics has been re-evaluated as the "classical limit" of quantum mechanics, and its more advanced developments in terms of quantum field theory, string theory, and speculative quantum gravity theories.

Quantum mechanics had enormous success in explaining many of the features of our world. It is often the only tool available that can reveal the individual behaviours of the subatomic particles that make up all forms of matter (electrons, protons, neutrons, photons, and others). Quantum mechanics is also critically important for understanding how individual atoms combine covalently to form molecules. The application of quantum mechanics to chemistry is known as quantum chemistry. Relativistic quantum mechanics can, in principle, mathematically describe most of chemistry. Quantum mechanics can also provide quantitative insight into ionic and covalent bonding processes by explicitly showing which molecules are energetically favourable to which others, and the magnitudes of the energies involved [13]. Furthermore, most of the calculations performed in modern computational chemistry rely on quantum mechanics.

A great deal of modern technological inventions operate at a scale where quantum effects are significant. Examples include the laser, the transistor (and thus the microchip), the electron microscope, and magnetic resonance imaging (MRI). The study of semiconductors led to the invention of the diode and the transistor, which are indispensable parts of modern electronics systems and devices.

Researchers are currently seeking robust methods of directly manipulating quantum states. Efforts are being made to more fully develop quantum cryptography, which will theoretically allow guaranteed secure transmission of information. A more distant goal is the development of quantum computers, which are expected to perform certain computational tasks exponentially faster than classical computers. Another active research topic is quantum teleportation, which deals with techniques to transmit quantum information over arbitrary distances.

Quantum tunneling is vital to the operation of many devices - even in the simple light switch, as otherwise the electrons in the electric current could not penetrate the potential barrier made up of a layer of oxide. Flash memory chips found in USB drives use quantum tunneling to erase their memory cells.

While quantum mechanics primarily applies to the atomic regimes of matter and energy, some systems exhibit quantum mechanical effects on a large scale - superfluidity, the frictionless flow of a liquid at temperatures near absolute zero, is one well-known example. Quantum theory also provides accurate descriptions for many previously unexplained phenomena, such as black body radiation and the stability of the orbitals of electrons in atoms. It has also given insight into the workings of many different biological systems, including smell receptors and protein structures [14]. Recent work on photosynthesis has provided evidence that quantum correlations play an essential role in this basic fundamental process of the plant kingdom [15]. Even so, classical physics can often provide good approximations to results otherwise obtained by quantum physics, typically in circumstances with large numbers of particles or large quantum numbers.

2.2 Wave - particle duality

Wave - particle duality postulates that all particles exhibit both wave and particle properties . A central concept of quantum mechanics, this duality addresses the inability of classical concepts like "particle" and "wave" to fully describe the behaviour of quantum-scale objects. Standard interpretations of quantum mechanics explain this paradox as a fundamental property of the Universe, while alternative interpretations explain the duality as an emergent, second-order consequence of various limitations of the observer. This treatment focuses on explaining the behaviour from the perspective of the widely used Copenhagen interpretation, in which wave - particle duality serves as one aspect of the concept of complementarity, that one can view phenomenon in one way or in another, but not both simultaneously.

The idea of duality originated in a debate over the nature of light and matter that dates back to the 17th century, when Christiaan Huygens and Isaac Newton proposed competing theories of light: light was thought either to consist of waves (Huygens) or of particles (Newton). Through the work of Max Planck, Albert Einstein, Louis de Broglie, Arthur Compton, Niels Bohr, and many others, current scientific theory holds that all particles also have a wave nature (and vice versa). This phenomenon has been verified not only for elementary particles, but also for compound particles like atoms and even molecules. For macroscopic particles, because of their extremely long wavelengths, wave properties usually cannot be detected

The relations that connect these two classically incompatible behaviours are the following

$$E = hf, \qquad p = \frac{h}{\lambda} \tag{2.2.1}$$

or, equivalently

$$f = \frac{E}{h}, \qquad \lambda = \frac{h}{p} \tag{2.2.2}$$

. In Eq. 2.2.1, the relations refer to whatever considered only as wave, i.e. the electromagnetic waves, and connect the wave features f and λ, the frequency and the wavelength respectively, with the particle features E and p, the energy and the momentum, respectively, of the particle. Similarly, the form in Eq. 2.2, the relations refer to whatever considered initially only as particle, i.e the electron, and connect the particle features with the wave features of the respective wave. The link between these two features, the wave and particle, is the Planck constant h If, instead of f and λ, we describe the waves with the use of the angular frequency and the wavenumber

$$\omega = \frac{2\pi}{T} = 2\pi f \quad and \quad k = \frac{2\pi}{\lambda}, \tag{2.2.3}$$

then form Eq. 2.2.1 we get

$$E = \hbar\omega, \qquad p = \hbar k \tag{2.2.4}$$

where $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant or Dirac constant. The above relations, Eq. 2.2.4, constitute the starting point of quantum mechanics, which will be asked to describe subatomic particles as particles and waves simultaneously.

2.3 Schrödinger Equation

The quantitative description of waves in classical mechanics requires a suitable wave equation. In the case of a mechanical wave, in three - dimensional space, this equation is of the form

$$\nabla^2 u - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = 0, \tag{2.3.1}$$

where $u = u(\boldsymbol{r}, t)$ is the displacement of the point $\boldsymbol{r}$ from the equilibrium point, at time t and

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{2.3.2}$$

is the Laplace operator or Laplacian.

Hence, a severe quantitative description of the material waves, waves that "accompany" the motion of the material particles, according to the wave - particle duality is not possible if a respective wave equation is not available. An equation should first devised and afterwards to check its legitimacy. The search of such an equation has been done by the Austrian physicist Erwin Schrödinger, who formulated in late 1925, and published in 1926 the so-called Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right)\psi \tag{2.3.3}$$

where m is the particle's mass, $V(\boldsymbol{r})$ is its potential energy, ∇^2 is the Laplacian, and $\psi = \psi(\boldsymbol{r}, t)$ is the wavefunction. The Schrödinger equation is a partial differential equation that describes how the quantum state of some physical system changes with time. In plain language, it means "total energy equals kinetic energy plus potential energy"

In classical mechanics, the equation of motion is Newton's second law, and equivalent formulations are the Euler Lagrange equations and Hamilton's equations. All of these formulations are used to solve for the motion of a mechanical system and mathematically predict what the system will do at any time beyond the initial settings and configuration of the system. In quantum mechanics, the analogue of Newton's law is Schrödinger's equation for a quantum system (usually atoms, molecules, and subatomic particles whether free, bound, or localized). It is not a simple algebraic equation, but (in general) a linear partial differential equation. The differential equation describes the wave function of the system, also called the quantum state or state vector.

In the standard interpretation of quantum mechanics, the wave function is the most complete description that can be given to a physical system. Solutions to Schrödinger's equation describe not only molecular, atomic, and subatomic systems, but also macroscopic systems, possibly even the whole universe [16]. Furthermore, Eq. 2.3.3 is written in the following form

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \tag{2.3.4}$$

where $\hat{H}$ is the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}). \tag{2.3.5}$$

The latter equation, Eq. 2.3.4 is known as the time-dependent Schrdinger equation, which gives a description of a system evolving with time.Here, an operator is a function acting on the space of physical states. As a result of its application on a physical state, another physical state is obtained, very often along with some extra relevant information. It is important to note that the operators used in quantum mechanics are linear and the application on a linear combination of wavefunctions is transferred on each function of the combination separately. To apply the Schrdinger equation, the Hamiltonian operator is set up for the system, accounting for the kinetic and potential energy of the particles constituting the system, then inserted into the Schrödinger equation. The resulting partial differential equation is solved for the wave function, which contains information about the system.

The time-dependent Schrödinger equation predicts that wave functions can form standing waves, called stationary states (also called "orbitals", as in atomic orbitals or molecular orbitals). These states are important in their own right, and moreover if the stationary states are classified and understood, then it becomes easier to solve the time-dependent Schrdinger equation for any state. The time-independent Schrödinger equation is the equation describing stationary states and it is only used when the Hamiltonian itself is not dependent on time. Its form is the following

$$E\psi = \hat{H}\psi \tag{2.3.6}$$

which states that when the Hamiltonian operator , $\hat{H}$, acts on the wave function ψ the result might be proportional to the same wave function ψ. If it is, then ψ is a stationary state, and the proportionality constant, E, is the energy of the state ψ. In linear algebra terminology, this equation is an eigenvalue equation, where E is the eigenvalue and ψ is the corresponding eigenvector.

Like Newton's Second law, the Schrödinger equation can be mathematically transformed into other formulations such as Werner Heisenberg's matrix mechanics, and Richard Feynman's path integral formulation. Also like Newton's Second law, the Schrödinger equation describes time in a way that is inconvenient for relativistic theories, a problem that is not as severe in matrix mechanics and completely absent in the path integral formulation. The equation is derived by partially differentiating the standard wave equation and substituting the relation between the momentum of the particle and the wavelength of the wave associated with the particle in De Broglie's hypothesis.

2.4 Dirac Notation

In quantum mechanics, bra - ket notation is a standard notation for describing quantum states, composed of angle brackets and vertical bars. It was introduced in 1939 by Paul Dirac [17] and is also known as Dirac notation, though the notation has precursors in Grassmann's use of the notation $[\psi|\psi]$ for his inner products nearly 100 years previously [18].

Two major mathematical traditions emerged in quantum mechanics; Heisenbergs matrix mechanics and Schrdingers wave mechanics. These distinctly different computational approaches to quantum theory are formally equivalent, each with its particular strengths in certain applications. Heisenbergs variation is based on matrix and vector algebra, while Schrdingers approach requires integral and differential calculus. Diracs notation can be used in a first step in which the quantum mechanical calculation is described or set up. Afterwards, one chooses either matrix or wave mechanics to complete the calculation, depending on which method is computationally the most expedient. In the recent work, the bra - ket or Dirac notation is used.

Bra ket formalism can also be used to denote abstract vectors and linear functionals in mathematics. It is so called because the inner product (or dot product on a complex vector space) of two states is denoted by a $\langle bra \,|\, ket \rangle$,

$$\langle \phi \,|\, \psi \rangle \,,$$

consisting of a left part, $\langle \phi |$, called the bra, and a right part, $| \psi \rangle$, called the ket.

This notation is widespread in quantum mechanics. Almost every phenomenon that is explained using quantum mechanics, including a large portion of modern physics, is usually explained with the help of this notation. Part of the appeal of the notation is the abstract representation - independence it encodes, together with its versatility in producing a specific representation (e.g., x, or p, or eigenfunction base) without much excessive reliance on the nature of the linear spaces involved. The overlap expression $\langle \phi \,|\, \psi \rangle$ is typically interpreted as the probability amplitude for the state ψ to collapse into the state ϕ.

Chapter 3

Density Matrix

3.1 Introduction

Density matrices, also called density operators, conceptually take the role of the state vectors as they encode all the accessible information about a quantum mechanical system. The notion of ensemble is an ingredient of the statistical interpretation of quantum mechanics. It describes the statistical distribution of quantum states in a system and allows to treat an ensemble of particles statistically. It turns out that the pure states, described by state vectors $|\psi\rangle$ on Hilbert space $\mathcal{H}$ (a complete, abstract vector space possessing the structure of an inner product that allows length and angle to be measured), are idealized descriptions that cannot characterize statistical (incoherent) mixtures, which often occur in the experiment. These objects are very important for the theory of quantum information and quantum communication.

3.2 General Properties

Consider an observable A in the pure state ψ with the expectation value given by

$$\langle A\rangle_\psi = \langle\psi\,|\,A\,|\,\psi\rangle \tag{3.2.1}$$

Then, the density matrix ρ for the pure state ψ is defined as

$$\rho := |\psi\rangle\,\langle\psi| \tag{3.2.2}$$

This density matrix has the following properties:

(a) $\rho^2 = \rho$, projector

(b) $\rho^\dagger = \rho$, hermicity

(c) $Tr(\rho) = 1$, normalization

(d) $\rho \geq 0$, positivity

From the last property (d) it follows that the eigenvalues of ρ are greater or equal to zero, which is important because probabilities are always greater or equal to zero. The expectation value of an observable in the state ψ can be reproduced and is given by

$$\langle A\rangle_\rho = Tr(A\rho) \tag{3.2.3}$$

3.3 Pure and Mixed States

Now we can introduce a broader class of states represented by density matrices, the mixed states in contrast to the states we have considered until now, the pure states.

3.3.1 Pure States

Consider an ensemble of given objects in the states $\{|\psi\rangle\}$. If all the objects are in the same state, the ensemble is represented by a pure state. To make probabilistic statements the whole ensemble of identically prepared systems must be considered.

Let the system be in the state ψ which can be expanded with respect to the eigenstates of a hermitian operator $\hat{A}$

$$|\psi\rangle = \sum_n c_n |n\rangle \ , \text{ where } \hat{A}|n\rangle = a_n |n\rangle \tag{3.3.1.1}$$

The expectation value is then given by

$$\left\langle \hat{A} \right\rangle_\psi = \sum_n |c_n|^2 a_n = \sum_n \frac{N_n}{N} a_n, \tag{3.3.1.2}$$

where $|c_n|^2$ is the probability to measure the eigenvalue a_n . It corresponds to the fraction N_n/N, the incidence the eigenvalue a_n occurs, where N_n is the number of times this eigenvalue has been measured out of an ensemble of N objects.

The state is characterized by a density matrix of the form of Eq. 3.2.2, with the same properties, where we can combine properties (c) and (d) to conclude $Tr(\rho^2) = 1$.

3.3.2 Mixed States

Let now study the situation where not all of the N systems (objects) of the ensemble are in the same state, for example N_i systems are in the state $|\psi_i\rangle$ respectively, such that $\sum N_i = N$.

While quantum measurement destroys the measured system, it is necessary to have available an entire collection of identical particles in order to make possible to check the theoretical statistical predictions by repeated measurements upon its unused members. This is succeeded by making use of the mean or expectation value equation Eq. 3.2.1, which summarize the physical content.

Hence, in practice all the ensembles that made available are not always pure. These ensembles consist of individual ones, each of them corresponding to a specific quantum state $|\psi_i\rangle$, different from the other states. Such a statistical mixture, a mixed ensemble, will be fully known if we know the participation rate $p_1, p_2, \ldots, p_N$ of the individual pure ensembles in it. This rates π_i are the probabilities if a random member of the full ensemble is described by the state $|\psi_i\rangle$. This probability p_i to find an individual system of the ensemble described by the state $|\psi_i\rangle$ is given by

$$p_i = \frac{N_i}{N}, \text{ where } \sum_i p_i = 1. \tag{3.3.2.1}$$

Thus we can express the mixed state as a convex sum (weighted sum with $\sum_i p_i = 1$) of pure state density matrices

$$\rho = \sum_i p_i \rho_i = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| \tag{3.3.2.2}$$

The expectation value is again given by Eq. 3.2.1 which we can express this as a convex sum of expectation values of its constituent pure states

$$\langle A\rangle_\rho = \sum_i p_i \left\langle \psi_i \,\middle|\, A \,\middle|\, \psi_i \right\rangle . \tag{3.3.2.3}$$

in the case of mixed states, the following properties hold for the density matrix

(a) $\rho^2 \neq \rho$

(b) $\rho^\dagger = \rho$

(c) $Tr(\rho) = 1$

(d) $\rho \geq 0$

(e) $Tr(\rho^2) < 1$

The trace of ρ^2, $Tr(\rho^2)$ is a good measure for the mixedness of a density matrix, since it is equal to 1 for pure states and strictly smaller than 1 for mixed states. For a maximally mixed state we have for a given dimension d of the system

$$Tr(\rho^2) = \frac{1}{d} > 0. \tag{3.3.2.4}$$

A simple example of a such a statistical mixture is a gas consisting of Hydrogen atoms in thermodynamic equilibrium in temperature T. This collection of atoms will be a mixed one, in which one part will be in the ground state, described by the state vector $|\psi_1\rangle$ and the other part will be in the excited state, described then by the state vector $|\psi_2\rangle$. The percentages of each part being in the corresponding state will be given by the Boltzmann equation

$$P_n = Ae^{-\,{E_n}/{k_B T}}, \tag{3.3.2.5}$$

where A is the normalization coefficient which is determined through the condition

$$\sum P_n = 1 \Rightarrow A = \frac{1}{e^{-\,{E_n}/{k_B T}}} = \frac{1}{Z} \tag{3.3.2.6}$$

where

$$Z = \sum_{n=1}^{\infty} e^{-\,{E_n}/{k_B T}} \tag{3.3.2.7}$$

is the partition function of the system.

3.4 Time Evolution of Density Matrices

Given the importance of the density matrix (or density operator) ρ, the next step is to investigate how it evolves with time. As to the nature of the statistical mixture, it is required to accept that the time evolution of all the states ψ_i, contained in the mixture, are governed by the same Hamiltonian, H. From the time-dependent Schrödinger equation and its hermitian conjugate

$$i\hbar\frac{\partial}{\partial t}\left|\psi_i(t)\right\rangle = H\left|\psi_i(t)\right\rangle \Rightarrow -i\hbar\frac{\partial}{\partial t}\left\langle\psi_i(t)\right| = \left\langle\psi_i(t)\right| H. \tag{3.4.1}$$

Then the differentiation of the equation-definition of the density matrix

$$\rho(t) = \sum_i p_i \left|\psi_i(t)\right\rangle \left\langle\psi_i(t)\right| \tag{3.4.2}$$

with respect to time will give

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\rho(t) &= \sum_i p_i \left(i\hbar\frac{\partial}{\partial t}\left|\psi_i(t)\right\rangle\right)\left\langle\psi_i(t)\right| + \sum_i p_i \left|\psi_i(t)\right\rangle\left(i\hbar\frac{\partial}{\partial t}\left\langle\psi_i(t)\right|\right)\\
&= \sum_i p_i H\left|\psi_i(t)\right\rangle\left\langle\psi_i(t)\right| + \sum_i p_i \left|\psi_i(t)\right\rangle\left(-\left\langle\psi_i(t)\right| H\right)\\
&= H\left(\sum_i p_i \left|\psi_i(t)\right\rangle\left\langle\psi_i(t)\right|\right) - \left(\sum_i p_i \left|\psi_i(t)\right\rangle\left\langle\psi_i(t)\right|\right)H\\
&= H\rho - \rho H\\
&= [H, \rho].
\end{aligned} \tag{3.4.3}$$

So, it holds that

$$i\hbar\frac{\partial}{\partial t}\rho(t) = [H, \rho(t)]. \tag{3.4.4}$$

This result denotes that the density matrices satisfy the von Neumann Equation, which is the quantum analogue to the classical Liouville equation.

The time evolution of the density matrix can be also described by applying a unitary operator, the time shift operator $U(t, t_0)$, also called propagator

$$U(t, t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}. \tag{3.4.5}$$

This allows to relate the density matrix at a later time t to the density matrix at some earlier time t_0

$$\rho(t) = U(t, t_0)\rho(t_0)U^\dagger(t, t_0). \tag{3.4.6}$$

Furthermore, it helps to prove, for instance, that the mixedness $Tr(\rho^2)$ of a density matrix is time independent

$$Tr(\rho^2(t)) = Tr(U\rho(t_0)U^\dagger U\rho(t_0)U^\dagger) = Tr(\rho(t_0)\rho(t_0)U^\dagger U) = Tr(\rho^2(t_0)) \tag{3.4.7}$$

where we used that $U^\dagger U = UU^\dagger = \mathbb{I}$ and the cyclic property of the trace operation, which is

$$Tr(ABCD) = Tr(BCDA) = Tr(CDAB) = Tr(DABC).$$

Chapter 4

Bloch or Coherence Vector

In quantum mechanics, the Bloch sphere (Poincar sphere in optics) is a geometrical representation of the pure state space of a two-level quantum mechanical system (qubit), named after the physicist Felix Bloch. There is a one-to-one correspondence between the states of a qubit and the points of a unit ball in $\mathbb{R}^3$ the Bloch ball. It has been generalized to systems with arbitrary number of levels. Unfortunately, for quantum systems with more than two levels, i.e for a three-level (qutrit), the correspondence is not so clear anymore as in the qubit case, because the subset of points of the Bloch ball that correspond to valid quantum states has a non trivial shape [1], [19]. But still the Bloch vectors provide a visual insight into the world of quantum states. Many operations on single qubits that are commonly used in quantum information processing can be neatly described within the Bloch sphere picture.

4.1 Two-Level System (Qubit)

Let's start with a simple definition of qubits. A qubit is a two-state quantum-mechanical system with basis states $|0\rangle = \begin{pmatrix}1 & 0\end{pmatrix}^T$ (ground state) and $|1\rangle = \begin{pmatrix}0 & 1\end{pmatrix}^T$ (excited state), as shown in Fig. 4.1. A pure qubit state is a linear superposition of the basis states, represented as a linear combination of the basis states:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \tag{4.1.1}$$

where α and β are probability amplitudes and can in general both be complex numbers. Also, the following relation holds:

$$|\alpha|^2 + |\beta|^2 = 1 \tag{4.1.2}$$

where $|\alpha|^2$ and $|\beta|^2$ are the probabilities of outcomes $|0\rangle$ and $|1\rangle$, respectively.
At this point, we will introduce the Bloch (or coherence) vector [1], [19] which will be useful for the solution of the Master Equation. In the case of qubits we use the $SU(2)$ unitary group. This group requires three linearly independent generators g_k which can be expressed in terms of the Pauli matrices σ_k with $k = 1, 2, 3$:

$$\sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\ \sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\ \sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{4.1.3}$$

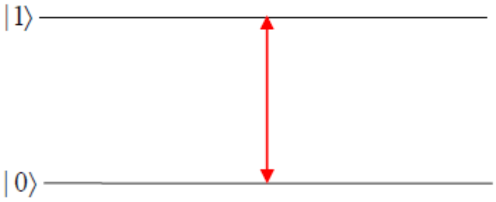


Figure 4.1: A two-level system (qubit) with basis states $|0\rangle$ and $|1\rangle$

The above matrices are hermitian, traceless and follow the following relations:

$$\begin{aligned} [\sigma_a, \sigma_b] &= \sum_c \varepsilon_{abc}\sigma_c \\ \{\sigma_a, \sigma_b\} &= 2\delta_{ab}\mathbb{I} \end{aligned} \tag{4.1.4}$$

where δ_{ab} is the Kronecker delta and ε_{abc} is the Levi-Civita symbol $(a, b, c = 1, 2, 3)$. Then, the Bloch vector $\mathbf{r}_b \in \mathbb{R}^3$, can be obtained through the relation:

$$\mathbf{r}_{b,k} = Tr(\rho\sigma_k), \quad k = 1, \dots, 3 \tag{4.1.5}$$

where ρ is the 2×2 density matrix and σ_k are the Pauli matrices. More analytically

$$\begin{aligned} \mathbf{r}_{b,1} &= \rho_{12} + \rho_{21} \\ \mathbf{r}_{b,2} &= i(\rho_{12} - \rho_{21}) \\ \mathbf{r}_{b,3} &= \rho_{11} - \rho_{22} \end{aligned} \tag{4.1.6}$$

Knowing the Bloch vector, we can express the density matrix as:

$$\rho_b = \frac{1}{2}(\mathbb{I} + \mathbf{r}_b \cdot \boldsymbol{\sigma}) \tag{4.1.7}$$

where $\mathbb{I}$ is the 2×2 identity matrix. From another perspective, unit Bloch sphere is a geometrical representation of the pure state space of a two-level quantum mechanical system (qubit). According to the length of this vector we can declare whether the states of the system are pure or mixed. So, if $|\mathbf{r}_b| = 1$ then we have pure states, if $|\mathbf{r}_b| < 1$ then we have mixed ones, otherwise if $|\mathbf{r}_b| = 0$ then he states are completely mixed.

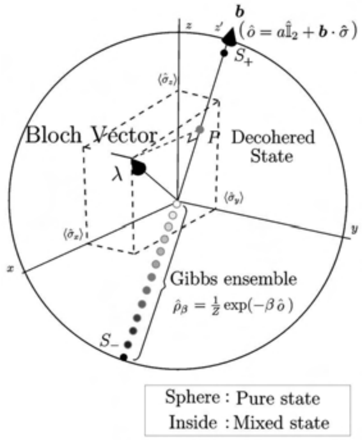


Figure 4.2: Bloch sphere in a two-level system (qubit) [1]

4.2 Three-Level System (Qutrit)

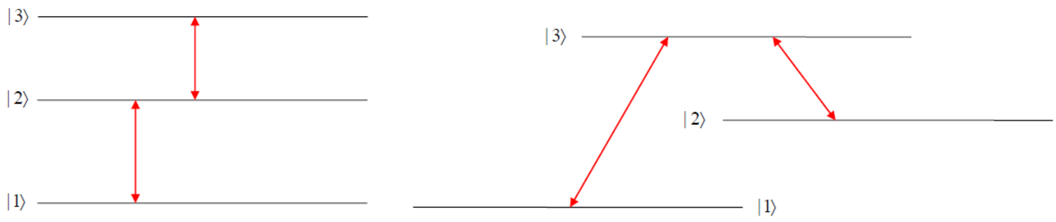
Similarly to qubit, a qutrit is a three-state quantum-mechanical system with basis states $|1\rangle = \begin{pmatrix}1 & 0 & 0\end{pmatrix}^T$ (ground state), $|2\rangle = \begin{pmatrix}0 & 1 & 0\end{pmatrix}^T$ (intermediate excited state) and $|3\rangle = \begin{pmatrix}0 & 0 & 1\end{pmatrix}^T$ (Rydberg excited state) and are usually studied in three configurations, as shown in Fig. 4.2.1. Each configuration has two dipole allowed transitions and one dipole forbidden transition, with the only difference being the relative arrangement of the energy levels. A pure qutrit state is a linear superposition of the basis states, represented as a linear combination of $|1\rangle$, $|2\rangle$ and $|3\rangle$:

$$|\psi\rangle = \alpha\,|1\rangle + \beta\,|2\rangle + \gamma\,|3\rangle \tag{4.2.1}$$

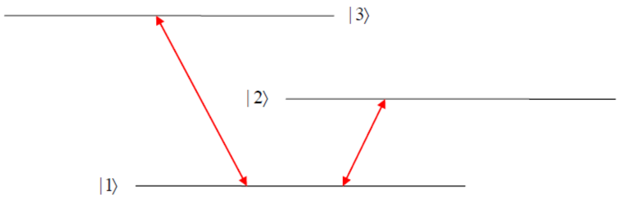
where α, β and γ are probability amplitudes and can in general both be complex numbers. As in qubit, the following relation should hold:

$$|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1 \tag{4.2.2}$$

where $|\alpha|^2$, $|\beta|^2$ and $|\gamma|^2$ are the probabilities of outcomes $|1\rangle$, $|2\rangle$ and $|3\rangle$, respectively.



(a) cascade or ladder (Ξ) **(b)** lamda (Λ)



(c) vee (V)

Figure 4.2.1: The three types of a three-level system (qutrit) with basis states $|1\rangle$, $|2\rangle$ and $|3\rangle$

Contrary to the qubit where we use the $SU(2)$ unitary group of dimension three, here we have the $SU(3)$ unitary group which is of dimension eight. This group requires eight linearly independent generators g_k which can be expressed in terms of the Gell-Mann matrices λ_k with $k = 1, \ldots, 8$ (two diagonals and six off-diagonals):

$$\begin{gathered}
\lambda_1 = \begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad \lambda_2 = \begin{pmatrix}0 & -i & 0\\ i & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad \lambda_3 = \begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 0\end{pmatrix}\\
\lambda_4 = \begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{pmatrix}, \quad \lambda_5 = \begin{pmatrix}0 & 0 & -i\\ 0 & 0 & 0\\ i & 0 & 0\end{pmatrix}, \quad \lambda_6 = \begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}\\
\lambda_7 = \begin{pmatrix}0 & 0 & 0\\ 0 & 0 & -i\\ 0 & i & 0\end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -2\end{pmatrix}
\end{gathered} \tag{4.2.3}$$

All matrices are hermitian, traceless and follow the following relations:

$$
\begin{aligned}
Tr(\lambda_a \lambda_b) &= 2\delta ab \\
[\lambda_a, \lambda_b] &= 2if_{abc}\lambda_c \\
\{\lambda_a, \lambda_b\} &= \frac{4}{3}\delta_{ab} + 2d_{abc}\lambda_c
\end{aligned}
\tag{4.2.4}
$$

where δ_{ab} is the Kronecker delta, d_{abc} are completely symmetric structure constants and f_{abc} are completely antisymmetric structure constants $(a, b, c = 1, \ldots, 8)$.

Now, the coherence vector in the case of qutrits [1], [19] $\mathbf{r}_t \in \mathbb{R}^8$ and can be obtained through the relation:

$$
\mathbf{r}_{t,k} = Tr(\rho\lambda_k), \;\; k = 1, \ldots, 8 \tag{4.2.5}
$$

where in this case ρ is the 3×3 density matrix and σ_k are the Pauli matrices. More analytically

$$
\begin{aligned}
\mathbf{r}_{t,1} &= \rho_{12} + \rho_{21} \\
\mathbf{r}_{t,2} &= i(\rho_{12} - \rho_{21}) \\
\mathbf{r}_{t,3} &= \rho_{11} - \rho_{22} \\
\mathbf{r}_{t,4} &= \rho_{13} + \rho_{31} \\
\mathbf{r}_{t,5} &= i(\rho_{13} - \rho_{31}) \\
\mathbf{r}_{t,6} &= \rho_{23} + \rho_{32} \\
\mathbf{r}_{t,7} &= i(\rho_{23} - \rho_{32}) \\
\mathbf{r}_{t,8} &= \frac{1}{\sqrt{3}}(\rho_{11} + \rho_{22} - \sqrt{2}\rho_{33})
\end{aligned}
\tag{4.2.6}
$$

Knowing the coherence vector $\mathbf{r}_t$, we can express the density matrix as:

$$
\rho_t = \frac{1}{3}(\mathbb{I} + \sqrt{3}\mathbf{r}_t \cdot \boldsymbol{\lambda}) \tag{4.2.7}
$$

where $\mathbb{I}$ is the 3×3 identity matrix.

As for the length of the coherence vector, for qutrits, if $|\mathbf{r}_t| = 1$ then we have pure states, otherwise if $|\mathbf{r}_b| < 1$ then we have mixed ones. It should be noticed that not all coherence vectors with $|\mathbf{r}_b| \leq 1$ correspond to valid qutrit states because a valid state has density matrix with non-negative eigenvalues. Also, the largest hypersphere, that contains only valid states has radius $|\mathbf{r}_b| = \frac{2}{3}$.

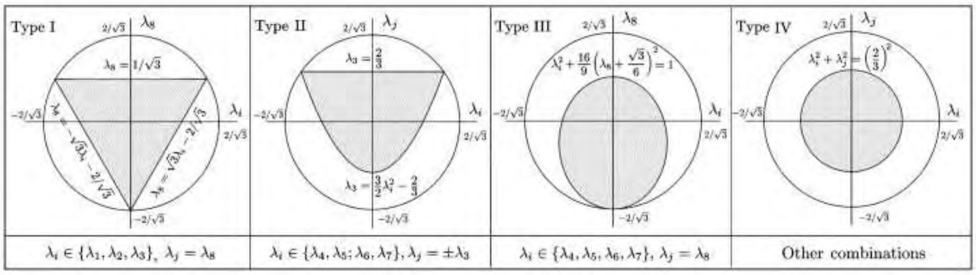


Figure 4.2.2: Two-dimensional sections of the Bloch (or Coherence) vector space for three-level systems. The grey parts are the domain of the Bloch vector. [1]

CHAPTER 5

QUANTUM MASTER EQUATIONS

5.1 Closed & Open Systems

5.1.1 Dynamics of Closed Quantum Systems

A closed quantum system a system that is closed in the sense that it does not interchange any information with another system (i.e. energy, particles, etc.). In physical applications one often encounters the situation that the system under consideration is driven by external forces, an external electromagnetic field for example. If in such a case the dynamics of the system can still be formulated in terms of a possibly time-dependent Hamiltonian generator $H(t)$ the system will again be said to be closed, while we reserve the term isolated to mean that the Hamiltonian of the system is time independent. The Planck's constant $\hbar$ has been set equal to 1.

The time evolution of a pure state $|\psi(t)\rangle \in \mathcal{H}$ generated by the Hamiltonian $H(t)$ is determined by the Schrödinger equation

$$\frac{d\,|\psi(t)\rangle}{dt} = -\frac{i}{\hbar}H(t)\,|\psi(t)\rangle\,, \tag{5.1.1.1}$$

.

Due to the linearity of the Schrödinger equation its solution is given by an evolution family $U(t, t_0)$ such that

$$|\psi(t)\rangle = U(t, t_0)\,|\psi(t_0)\rangle\,, \tag{5.1.1.2}$$

where $U(t, t_0)$ is a unitary time-evolution operator, i.e. $U^\dagger(t, t_0)U(t, t_0) = U(t, t_0)U^\dagger(t, t_0) \equiv \mathbb{I}$, which transforms the state $|\psi(t_0)\rangle$ at some initial time t_0 to the state $|\psi(t)\rangle$ at time t. If we substitute Eq. 5.1.1.2 into Eq. 5.1.1.1 we get an operator equation for the time-evolution for $U(t, t_0)$

$$\frac{dU(t, t_0)}{dt} = -\frac{i}{\hbar}[H(t), U(t, t_0)]. \tag{5.1.1.3}$$

which is subjected to the initial condition

$$U(t_0, t_0) = \mathbb{I}. \tag{5.1.1.4}$$

For a closed, isolated physical system the Hamiltonian H is time independent and Eq. 5.1.1.3 is readily integrated to yield the following expression

$$U(t, t_0) = e^{-iH(t-t_0)}. \tag{5.1.1.5}$$

For a time-dependent Hamiltonian the solution of Eq. 5.1.1.3 subjected to the initial condition 5.1.1.4 represented as a time-ordered exponential

$$U(t,t_0) = T_{\leftarrow} exp\left(-i\sum_{t_0}^{t} dsH(s)\right) \tag{5.1.1.6}$$

where $T_{\leftarrow}$ denotes the chronological time-ordering operator which orders products of time-dependent operators such that their time-arguments increase from right to left as indicated by the arrow.

If the system under consideration is in a mixed state the corresponding quantum statistical ensemble may be characterized with the help of the statistical operator ρ. Assuming that at some initial time t_0 the state of the system is described by the density matrix

$$\rho(t_0) = \sum_{\alpha} w_\alpha \left|\psi_\alpha(t0)\right\rangle \left\langle\psi_\alpha(t0)\right|, \tag{5.1.1.7}$$

where w_α are positive weights and $ket\psi_\alpha(t0)$ are normalized state vectors. The state of the system at time t will therefore be given by

$$\rho(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0). \tag{5.1.1.8}$$

In this case, the time evolution of a mixed state, $\rho(t)$, is determined by the Liouville - von Neumann equation

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H(t),\rho(t)]. \tag{5.1.1.9}$$

which is often written in a form analogous to the classical Liouville equation

$$\frac{d\rho(t)}{dt} = \mathcal{L}(t)\rho(t). \tag{5.1.1.10}$$

Here, $\mathcal{L}$ is the Liouville operator is defined through the condition that

$$\mathcal{L}(t)\rho(t) = -i[H(t),\rho(t)]. \tag{5.1.1.11}$$

Often, $\mathcal{L}$ is called a Liouville superoperator since it acts on an operator to yield another operator. In close analogy with Eq. 5.1.1.6 the Liouville equation 5.1.1.10 leads to

$$\rho(t) = T_{\leftarrow} exp\left(\sum_{t_0}^{t} ds\mathcal{L}(s)\right)\rho(t_0). \tag{5.1.1.12}$$

For the case of a time independent Hamiltonian the Liouville superoperator is also time independent and hence we have

$$\rho(t) = e^{\mathcal{L}(t-t_0)}\rho(t_0). \tag{5.1.1.13}$$

5.1.2 Dynamics of Open Systems

In general terms, an open system is a quantum system S which is coupled to another quantum system B called the environment. It thus represents a subsystem of the combined total system $S+B$, whereby in most cases it is assumed that the combined system is closed, following Hamiltonian dynamics. The state of the subsystem S, however, will change as a consequence of its internal dynamics and of the interaction with the surroundings. The interaction leads to certain system-environment correlations such that the resulting state changes of S can no longer, in general, be represented in terms of unitary, Hamiltonian dynamics. The dynamics of the subsystem S induced by the Hamiltonian evolution of the total system is often referred to as reduced system dynamics, and S is also called the reduced system. Let us denote by $\mathcal{H}_S$, the Hilbert space of the system and by $\mathcal{H}_B$ the Hilbert space of the environment. The Hilbert space of the total system $S+B$ is then given by the tensor product space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$. The total Hamiltonian $H(t)$ may be taken to be of the form

$$H(t) = H_S \otimes I_B + I_S \otimes H_B + H_I(t) \tag{5.1.2.1}$$

where H_S is the self-Hamiltonian of the open system S, H_B is the free Hamiltonian of the environment B, and $H_I(t)$ is the Hamiltonian describing the interaction between the system and the environment. A schematic picture of the typical situation under study is shown in Fig. 5.1.1 Following the notation in [2], if we speak of an open system S we shall use the general term environment for the system B coupled to it. The term reservoir refers to an environment with an infinite number of degrees of freedom such that the frequencies of the reservoir modes form a continuum. As will be seen, it is this property which generally leads to an irreversible behaviour of the open quantum system. Finally, the term bath or heat bath will be used for a reservoir which is in a thermal equilibrium state.

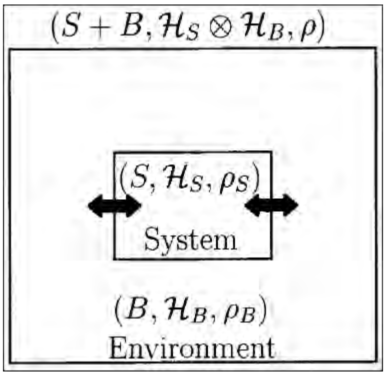


Figure 5.1.1: Schematic picture of an open quantum system. [2]

The motivation for the study of open systems is mainly that in many physically important situations a complete mathematical model of the combined system's dynamics is much too complicated. The environment may represent, for example, a reservoir or a heat bath consisting of infinitely many degrees of freedom, in which case an exact treatment requires the solution of an infinite hierarchy of coupled equations of motion. Even if a solution is known one is confronted with the task of isolating and determining the interesting physical quantities through an average over the remaining, irrelevant degrees of freedom. Moreover, one often encounters the situation that the modes of the environment are neither known exactly nor controllable. One therefore tries to develop a simpler description in a reduced state space formed by a restricted set of physically relevant variables which is achieved by employing various analytical methods and approximation techniques.

We regard an open system S to be singled out by the fact that all observations of interest refer to this subsystem. The observables referring to S are all of the form $A \otimes I_B$, where A is an operator acting on the Hilbert space $\mathcal{H}_S$ and I_B denotes the identity in the Hilbert space $\mathcal{H}_B$. If the state of the total system is described by some density matrix ρ, then the expectation values of all observables acting on the open system's Hilbert space are determined through

$$\langle A \rangle = Tr_S(A\rho_S), \tag{5.1.2.2}$$

where

$$\rho_S = Tr_B(\rho) \tag{5.1.2.3}$$

is the reduced density matrix of the open quantum system S. The notation Tr_S denotes the partial trace over the open system's Hilbert space, while Tr_B denotes the partial trace over the degrees of freedom of the environment B. The reduced density operator ρ_S will be the quantity of central interest in the description of open quantum systems.

The reduced density matrix $\rho_S(t)$ at time t is obtained from the density matrix $\rho(t)$ of the total system by taking the partial trace over the degrees of freedom of the environment. Since the total density matrix evolves unitarily we have

$$\rho_S(t) = Tr_B\left(U(t,t_0)\rho(t_0)U^\dagger(t,t_0)\right), \tag{5.1.2.4}$$

where $U(t,t_0)$ is the time-evolution operator of the total system. In an analogous way, the equation of motion for the reduced density matrix is obtained by taking the partial trace over the environment on both sides of the Liouville - von Neumann equation for the total system,

$$\frac{d\rho_S(t)}{dt} = -iTr_B[H(t),\rho(t)]. \tag{5.1.2.5}$$

5.2 Lindblad Quantum Master Equation

The general Lindblad form of a master equation is given by equation 5.2.1, where H is the Hamiltonian, which is Hermitian, and $\{A_k\}$ are so-called Lindblad operators such that for every operator its hermitian conjugate is also in the set labelled by k. The constants $\gamma_k \geq 0$ are called decay constants.

$$\frac{d\rho(t)}{dt} = -i[H,\rho(t)] + \sum_k \gamma_k \left[A_k\rho(t)A_k^\dagger - \frac{1}{2}\{A_k^\dagger A_k,\rho(t)\}\right] \tag{5.2.1}$$

Introducing superoperators we can write the Lindblad quantum master equation as

$$\mathcal{L}\rho(t) = -i[H,\rho(t)] + \mathcal{D}\rho(t) \tag{5.2.2}$$

where $\mathcal{L}$ is called the Lindbladian and $\mathcal{D}$ is the Dissipator.

5.3 Microscopic Derivations

5.3.1 Weak-Coupling Limit

We begin by considering a quantum mechanical system S weakly coupled to a reservoir B. The Hamiltonian of the total system is assumed to be of the form

$$H = H_S + H_B + H_I \tag{5.3.1.1}$$

where H_S and H_B denote respectively the free Hamiltonian of the system and of the reservoir and H_I describes the interaction between the system and the reservoir. The derivation of a quantum Markovian master equation is most easily performed in the interaction picture. The starting point is the interaction picture von Neumann equation

$$\frac{d\rho(t)}{dt} = -i[H_I(t), \rho(t)] \tag{5.3.1.2}$$

for the total density matrix $\rho(t)$ and its integral form

$$\rho(t) = \rho(0) - i \int_0^t ds[H_I(s), \rho(s)]. \tag{5.3.1.3}$$

Inserting the integral form into Eq. 5.3.1.2 and taking the trace over the reservoir we find

$$\frac{d\rho_S(t)}{dt} = - \int_0^t dsTr_B[H_I(t), [H_I(s), \rho(s)]]. \tag{5.3.1.4}$$

Here, it has been assumed that

$$Tr_B[H_I(t), \rho(0)] = 0. \tag{5.3.1.5}$$

In Eq. 5.3.1.4 still there is the density matrix of the total system, $\rho(t)$ on right-hand side. In order to eliminate it from the equation of motion we perform a first approximation, known as the Born approximation. This approximation assumes that the coupling between the system and the reservoir is weak, such that the influence of the system on the reservoir is small (weak-coupling approximation). Thus, the density matrix of the reservoir ρ_B is only negligibly affected by the interaction and the state of the total system at time t may be approximately characterized by a tensor product

$$\rho(t) \approx \rho_S(t) \otimes \rho_B. \tag{5.3.1.6}$$

Note that this does not imply that there are no excitations in the reservoir caused by the reduced system. The Markovian approximation to be derived below provides a description on a coarse-grained time scale and the assumption is that environmental excitations decay over times which are not resolved. Inserting the tensor product into the exact equation of motion, Eq.5.3.1.4, we obtain a closed integro-differential equation for the reduced density matrix $\rho_S(t)$

$$\frac{d\rho_S(t)}{dt} = - \int_0^t dsTr_B[H_I(t), [H_I(s), \rho_S(s) \otimes \rho_B]]. \tag{5.3.1.7}$$

In order to simplify the above equation we perform the Markov approximation, in which the integrand $\rho_S(s)$ is first replaced by $\rho_S(t)$. In this way we obtain an equation of motion for the reduced system's density matrix in which the time development of the state of the system at time t only depends on the present state $\rho_S(t)$,

$$\frac{\rho_S(t)}{dt} = - \int_0^t dsTr_B[H_I(t), [H_I(s), \rho_S(t) \otimes \rho_B]]. \tag{5.3.1.8}$$

This equation is called the Redfield equation [20], [21].

The Redfield equation is local in time, but it is not yet a Markovian master equation since the time evolution of the reduced density matrix still depends upon an explicit choice for the initial preparation at time $t = 0$. This implies that the dynamics of the reduced system is not yet described by a dynamical semigroup. In order to achieve this we substitute s by $t-s$ in the integral in Eq. 5.3.1.8 and let the upper limit of the integral go to infinity. This is permissible provided the integrand disappears sufficiently fast for $s >> \tau_B$. The Markov approximation is therefore justified if the time scale τ_R over which the state of the system varies appreciably is large compared to the time scale τ_B over which the reservoir correlation functions decay. Thus, we finally obtain the Markovian quantum master equation

$$\frac{d\rho_S(t)}{dt} = -\int_0^\infty ds Tr_B[H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]]. \tag{5.3.1.9}$$

The approximations performed above are usually termed as the Born-Markov approximation. In general they do not guarantee, however, that the resulting equation, Eq. 5.3.1.9 defines the generator of a dynamical semigroup ([22]). One therefore performs a further secular approximation which involves an averaging over the rapidly oscillating terms in the master equation and is known as the rotating wave approximation (RWA). To explain the procedure let us write the Schrödinger picture interaction Hamiltonian H_I in the form

$$H_I = \sum_\alpha A_\alpha \otimes B_\alpha, \tag{5.3.1.10}$$

where $A_\alpha^\dagger = A_\alpha$ and $B_\alpha^\dagger = B_\alpha$. This is the more general form of the interaction. In order to apply the this approximation, the interaction Hamiltonian, H_I, should be decomposed into eigenoperators of the system Hamiltonian, H_S. Supposing the spectrum of H_S to be discrete this may be achieved as follows. Let us denote the eigenvalues of H_S by ε and the projection onto the eigenspace belonging to the eigenvalue ε by $\Pi(\varepsilon)$. Then we can define the operators

$$A_\alpha(\omega) \equiv \sum_{\varepsilon' - \varepsilon = \omega} \Pi(\varepsilon) A_\alpha \Pi(\varepsilon'). \tag{5.3.1.11}$$

The above sum is extended over all energy eigenvalues ε' and ε of H_S with a fixed energy difference of ω. An immediate consequence of this definition is that the following relations are satisfied,

$$[H_S, A_\alpha(\omega)] = -\omega A_\alpha(\omega), \tag{5.3.1.12a}$$

$$[H_S, A_\alpha^\dagger(\omega)] = -\omega A_\alpha^\dagger(\omega). \tag{5.3.1.12b}$$

The operators $A_\alpha(\omega)$ and $A_\alpha^\dagger(\omega)$ are therefore said to be eigenoperators of H_S belonging to the frequencies $+\omega$ and $-\omega$, respectively. It follows from relations 5.3.1.12a and 5.3.1.12b that the corresponding interaction picture operators take the form

$$e^{iH_S t} A_\alpha(\omega) e^{-iH_S t} = e^{-i\omega t} A_\alpha(\omega), \tag{5.3.1.13a}$$

$$e^{iH_S t} A_\alpha^\dagger(\omega) e^{-iH_S t} = e^{-i\omega t} A_\alpha^\dagger(\omega). \tag{5.3.1.13b}$$

Finally, we note that

$$[H_S, A_\alpha^\dagger(\omega) A_\beta^\dagger(\omega)] = 0, \tag{5.3.1.14}$$

and

$$A^{\dagger}_{\alpha}(\omega) = A_{\alpha}(-\omega). \tag{5.3.1.15}$$

Summing Eq. 5.3.1.11 over all energy differences and employing the completeness relation we get

$$\sum_{\omega} A_{\alpha}(\omega) = \sum_{\omega} A^{\dagger}_{\alpha}(\omega) = A_{\alpha}. \tag{5.3.1.16}$$

This enables to cast the interaction Hamiltonian into the following form

$$H_I = \sum_{\alpha,\omega} A_{\alpha}(\omega) \otimes B_{\alpha} = \sum_{\alpha,\omega} A^{\dagger}_{\alpha}(\omega) \otimes B^{\dagger}_{\alpha}. \tag{5.3.1.17}$$

This is the desired decomposition of the interaction into eigenoperators of the system Hamiltonian. Note that the frequency spectrum $\{\omega\}$ is, in general, degenerate; for a fixed ω the index α labels the different operators $A_{\alpha}(\omega)$ belonging to the same frequency. By introducing this eigenoperator decomposition, the interaction picture interaction Hamiltonian can now be written in the particularly simple form

$$H_I(t) = \sum_{\alpha,\omega} e^{-i\omega t} A_{\alpha}(\omega) \otimes B_{\alpha}(t) = \sum_{\alpha,\omega} e^{+i\omega t} A^{\dagger}_{\alpha}(\omega) \otimes B^{\dagger}_{\alpha}(t), \tag{5.3.1.18}$$

where

$$B_{\alpha}(t) = e^{iH_B t} B_{\alpha} e^{-iH_B t} \tag{5.3.1.19}$$

are interaction picture operators of the environment. Now, the condition in Eq. 5.3.1.5 becomes

$$\langle B_{\alpha}(t) \rangle = Tr(B_{\alpha}(t)\rho_B = 0, \tag{5.3.1.20}$$

which states that the reservoir averages of the $B_{\alpha}(t)$ vanish. Inserting Eq. 5.3.1.18 into the master equation, Eq. 5.3.1.9 we obtain

$$\begin{aligned} \frac{d\rho_S(t)}{dt} &= \int_0^{\infty} ds Tr_B \left(H_I(t-s)\rho_S(t)\rho_B(t)H_I(t) - H_I(t)H_I(t-s)\rho_S(t)\rho_B\right) + h.c. \\ &= \sum_{\omega,\omega'} \sum_{\alpha,\beta} e^{i(\omega'-\omega)} \Gamma_{\alpha,\beta}(\omega) \left(A_{\beta}(\omega)\rho_S(t) A^{\dagger}_{\alpha'} - A^{\dagger}_{\alpha'} A_{\beta}(\omega)\rho_S(t) \right) + h.c. \end{aligned} \tag{5.3.1.21}$$

where h.c stands for the Hermitian conjugate expression and also have been introduced the one-side Fourier transforms

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^{\infty} ds e^{I\omega s} \left\langle B^{\dagger}_{\alpha}(t) B_{\beta}(t-s) \right\rangle \tag{5.3.1.22}$$

of the reservoir correlation functions

$$\left\langle B^{\dagger}_{\alpha}(t) B_{\beta}(t-s) \right\rangle \equiv Tr_B\{B^{\dagger}_{\alpha}(t) B_{\beta}(t-s)\rho_B\}. \tag{5.3.1.23}$$

Supposing that ρ_B is a stationary state of the reservoir, we get that $[H_B, \rho_B] = 0$. The reservoir correlation functions are then homogeneous in time which yields

$$\left\langle B^{\dagger}_{\alpha}(t) B_{\beta}(t-s) \right\rangle = \left\langle B^{\dagger}_{\alpha}(s) B_{\beta}(0) \right\rangle \tag{5.3.1.24}$$

showing that the quantities $\Gamma_{\alpha\beta}$ do not depend on time. An interesting example in which the reservoir correlation functions do depend on the time argument t is the case where the reservoir represents a squeezed vacuum state [2]. The basic condition underlying the Markov approximation is that the reservoir correlation functions 5.3.1.24 decay sufficiently fast over a time τ_B which is small compared to the relaxation time τ_R. It is important to note that a decay of the correlations can only be strictly valid for an environment which is infinitely large and involves a continuum of frequencies. If the frequency spectrum ω_n of the reservoir modes is discrete, it is easy to see that, in general, correlation functions of the type 5.3.1.24 are quasi-periodic functions of s. A rapid decay of the reservoir correlations therefore requires a continuum of frequencies. We denote by τ_S the typical time scale of the intrinsic evolution of the system S. This time scale T_S is defined by a typical value for $|\omega' - \omega|^{-1}$, $\omega' \neq \omega$, that is by a typical value for the inverse of the frequency differences involved. If τ_S is large compared to the relaxation time τ_R of the open system the non-secular terms in 5.3.1.21, i.e. the terms for which $\omega' \neq \omega$, may be neglected, since they oscillate very rapidly during the time τ_R over which ρ_S varies appreciably. This condition is typically satisfied for quantum optical systems where it is known as the rotating wave approximation (RWA). Thus we have

$$\frac{d\rho_S(t)}{dt} = \sum_{\omega}^{\alpha,\beta} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega)\rho_S(t)A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega)A_\beta(\omega)\rho_S(t) \right) + h.c. \qquad (5.3.1.25)$$

It is convenient to decompose the Fourier transforms of the reservoir correlation functions as follows

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + iS_{\alpha\beta}(\omega), \qquad (5.3.1.26)$$

where for fixed ω the coefficients

$$S_{\alpha\beta}(\omega) = \frac{1}{2i}(\Gamma_{\alpha\beta}(\omega) - \Gamma^*_{\beta\alpha}(\omega)) \qquad (5.3.1.27)$$

form a Hermitian matrix and the matrix defined by

$$\gamma_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma^*_{\beta\alpha}(\omega) = \int_{-\infty}^{+\infty} ds e^{i\omega s} \left\langle B_\alpha^\dagger(s)B_\beta(0) \right\rangle \qquad (5.3.1.28)$$

is positive. With these definitions we finally arrive at the interaction picture master equation

$$\frac{d\rho_S(t)}{dt} = -i[H_{LS}, \rho_S(t)] + \mathcal{D}(\rho_S(t)). \qquad (5.3.1.29)$$

The Hermitian operator

$$H_{LS} = \sum_{\omega}^{\alpha,\beta} S_{\alpha\beta}(\omega)A_\alpha^\dagger(\omega)A_\beta(\omega) \qquad (5.3.1.30)$$

provides a Hamiltonian contribution to the dynamics. This term is often called the Lamb shift Hamiltonian since it leads to a Lamb-type renormalization of the unperturbed energy levels induced by the system-reservoir coupling. Note that the Lamb shift Hamiltonian commutes with the unperturbed system Hamiltonian,

$$[H_S, H_{LS}] = 0. \qquad (5.3.1.31)$$

by virtue of Eq. 5.3.1.14. Finally, the dissipator of the master equation takes the form

$$\mathcal{D}(\rho_S) = \sum_{\omega} \sum_{\alpha,\beta} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega)\rho_S A_\alpha^\dagger(\omega) - \frac{1}{2}\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_S\} \right). \tag{5.3.1.32}$$

Note that the master equation 5.3.1.29 is of the first standard form

$$\mathcal{L}\rho_S = -i[H, \rho_S] + \sum_{i,j=1}^{N^2-1} \alpha_{ij} \left(F_i \rho_S F_j^\dagger - \frac{1}{2}\{F_j^\dagger F_i, \rho_S\} \right) \tag{5.3.1.33}$$

and can be brought into the Lindblad (diagonal) form

$$\mathcal{L}\rho_S = -i[H, \rho_S] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S A_k^\dagger - \frac{1}{2}\{A_k^\dagger A_k, \rho_S\} \right) \tag{5.3.1.34}$$

by diagonalization of the matrices $\gamma_{\alpha\beta}$.

5.4 Projector Operator Technique

We consider the general physical situation of an open system S coupled to an environment B. The dynamics of the density matrix $\rho(t)$ of the combined system is specified by some microscopic Hamiltonian of the form

$$H = H_0 + \alpha H_I \tag{5.4.1}$$

where H_0 generates the uncoupled time evolution of the system and environment. H_I describes their interaction, and α denotes a dimensionless expansion parameter. When working in the interaction representation, the equation of motion for the density matrix reads

$$\frac{\partial \rho(t)}{\partial t} = -i\alpha[H_I(t), \rho(t)] \equiv \alpha\mathcal{L}(t)\rho(t) \tag{5.4.2}$$

where we have set $\hbar = 1$ and the interaction picture representation of the interaction Hamiltonian is defined by

$$H_I(t) = e^{iH_0 t} H_I e^{-iH_0 t} \tag{5.4.3}$$

The Liouville super-operator is denoted by $\mathcal{L}(t)$.

5.4.1 Projection Operators

In order to derive an exact equation of motion for the reduced density matrix ρ_S of the open system it is convenient to define a super-operator $\mathcal{P}$ according to

$$\rho \mapsto \mathscr{P}\rho = Tr_B(\rho) \otimes \rho_B \equiv \rho_S \otimes \rho_B \tag{5.4.1.1}$$

where ρ_B is some fixed state of the environment. This super-operator projects on the relevant part of the density matrix ρ in the sense that $\mathcal{P}\rho$ gives the complete information required to reconstruct the reduced density matrix ρ_S of the open system. Accordingly, a complementary super-operator $\mathscr{Q}$,

$$\mathscr{Q}\rho = \rho - \mathcal{P}\rho \tag{5.4.1.2}$$

may be introduced, which projects on the irrelevant part of the density matrix. The super-operators $\mathscr{P}$ and $\mathscr{Q}$ are maps in the state space of the combined system that is in the space of density matrices of the total Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$. They have the following properties

$$\mathscr{P} + \mathscr{Q} = \mathbb{I} \tag{5.4.1.3}$$

$$\mathscr{P}^2 = \mathscr{P} \tag{5.4.1.4}$$

$$\mathscr{Q}^2 = \mathscr{Q} \tag{5.4.1.5}$$

$$\mathscr{P}\mathscr{Q} = \mathscr{Q}\mathscr{P} = 0 \tag{5.4.1.6}$$

which can be carried out using Eqs 5.4.1.1, 5.4.1.2 and assuming ρ_B to be normalized, $Tr(\rho_B) = 1$. The density matrix ρ_B used in Eq. 5.4.1.1 is an operator in $\mathcal{H}_B$. It may represent a quite arbitrary, but known environmental state, called the reference state. The choice of ρ_B strongly depends on the specific application one has in mind. In the following we shall suppose this state to be time independent. Typically, it is taken to be the stationary Gibbs state of the environment.

5.4.2 The Nakajima - Zwanzig equation

Our aim is now to derive a closed equation for the relevant part $\mathscr{P}\rho(t)$, i.e. for the density matrix $\rho_S(t) = Tr_B\rho(t)$ of the open system. By applying the projection operators $\mathscr{P}$ and $\mathscr{Q}$ to the Liouville-von Neumann equation, Eq. 5.4.2, and by invoking the time independence of the reference state the following set of coupled differential equations for the relevant and the irrelevant part of the density matrix is obtained,

$$\frac{\partial \mathscr{P}\rho(t)}{\partial t} = \mathscr{P}\frac{\partial \rho(t)}{\partial t} = \alpha \mathscr{P}\mathcal{L}(t)\rho(t) \tag{5.4.2.1}$$

$$\frac{\partial \mathscr{Q}\rho(t)}{\partial t} = \mathscr{Q}\frac{\partial \rho(t)}{\partial t} = \alpha \mathscr{Q}\mathcal{L}(t)\rho(t) \tag{5.4.2.2}$$

By inserting the identity $\mathbb{I} = \mathcal{P} + \mathcal{Q}$ between the Liouville operator and the density matrix ρ this may also be written as

$$\frac{\partial \mathscr{P}\rho(t)}{\partial t} = \alpha \mathscr{P}\mathcal{L}(t)\mathscr{P}\rho(t) + \alpha \mathscr{P}\mathcal{L}(t)\mathscr{Q}\rho(t) \tag{5.4.2.3}$$

$$\frac{\partial \mathscr{Q}\rho(t)}{\partial t} = \alpha \mathscr{Q}\mathcal{L}(t)\mathscr{P}\rho(t) + \alpha \mathscr{Q}\mathcal{L}(t)\mathscr{Q}\rho(t) \tag{5.4.2.4}$$

To get a closed equation for the relevant part of the density matrix we solve Eq. 5.4.2.4 and insert the solution into Eq. 5.4.2.3. The formal solution of 5.4.2.4 corresponding to a given $\rho(t_0)$ at some initial time t_0 may be expressed as

$$\mathscr{Q}\rho(t) = \mathscr{G}(t, t_0)\mathscr{Q}\rho(t_0) + \alpha \int_{t_0}^{t} ds \mathscr{G}(t, s)\mathscr{Q}\mathcal{L}(s)\mathscr{P}\rho(s) \tag{5.4.2.5}$$

where we have introduced the propagator

$$\mathscr{G}(t, s) \equiv T_{\leftarrow} e^{\alpha \int_{s}^{t} ds' \mathscr{Q}\mathcal{L}}(s') \tag{5.4.2.6}$$

The operator $T_{\leftarrow}$, describes the chronological time ordering; it orders any product of super-operators such that the time arguments increase from right to left. The propagator $\mathscr{G}(t,s)$ thus satisfies the differential equation

$$\frac{\partial \mathscr{G}(t,s)}{\partial t} = \alpha \mathscr{Q}\mathcal{L}(t)\mathscr{G}(t,s) \tag{5.4.2.7}$$

with the initial condition

$$\mathscr{G}(s,s) = \mathbb{I} \tag{5.4.2.8}$$

Inserting the expression 5.4.2.5 for the irrelevant part of the density matrix into the equation of motion 5.4.2.3 for the relevant part we obtain the desired exact equation for the time evolution of the relevant part of the density matrix.

$$\begin{aligned}\frac{\partial \mathscr{P}\rho(t)}{\partial t} =& \alpha \mathscr{P}\mathcal{L}(t)\mathscr{G}(t,t_0)\mathscr{Q}\rho(t_0) + \alpha \mathscr{P}\mathcal{L}(t)\mathscr{P}\rho(t) \\ &+ \alpha^2 \int_{t_0}^{t} ds \mathscr{P}\mathcal{L}(t)\mathscr{G}(t,t_0)\mathscr{Q}\mathcal{L}(s)\mathscr{P}\tilde{\rho}_S\end{aligned} \tag{5.4.2.9}$$

This equation is known as the Nakajima - Zwanzig equation. It is an exact equation for the relevant degrees of freedom of the reduced system. The right-hand side involves an inhomogeneous term $\mathscr{P}\mathcal{L}(t)\mathscr{G}(t,t_0)\mathscr{Q}\rho(t_0)$ depending on the initial condition at time t_0, and an integral over the past history of the system in the time interval $[t_0,t]$. It thus describes completely non - Markovian (i.e memoryless) memory effects of the reduced dynamics. In many cases it may also be assumed that the odd moments of the interaction Hamiltonian with respect to the reference state vanish

$$Tr_B\left(H_I(t_1)H_I(t_2)\dots H_I(t_{2n+1}) = 0\right) \tag{5.4.2.10}$$

which leads to the following relation

$$\mathscr{P}\mathcal{L}(t_1)\mathcal{L}(t_2)\dots\mathcal{L}(t_{2n+1}\mathscr{P} = 0 \tag{5.4.2.11}$$

for $n = 0, 1, 2, \dots$. In the case where $n = 0$, the second term in the Nakajima - Zwanzig equation 5.4.2.9 vanishes and we may cast it into the compact form

$$\frac{d\mathscr{P}\rho(t)}{dt} = \int_{t_0}^{t} ds \mathscr{K}(t,s)\mathscr{P}\rho(s) + \alpha \mathscr{P}\mathcal{L}(t)\mathscr{G}(t,t_0)\mathscr{Q}\rho(t_0) \tag{5.4.2.12}$$

The convolution or memory kernel

$$\mathscr{K}(t,s) = \alpha^2 \mathscr{P}\mathcal{L}(t)\mathscr{G}(t,s)\mathscr{Q}\mathcal{L}(s)\mathscr{P} \tag{5.4.2.13}$$

represents a super-operator in the relevant subspace. The integro-differential equation5.4.2.12 is exact and holds for all initial conditions and for almost arbitrary systems and interactions. Unfortunately, the NakajimaZwanzig equation is usually as difficult to solve as the Liouville equation describing the dynamics of the total system [2]. This means that perturbation expansions are needed in order to discuss the relevant dynamics in a way accessible to analytical or numerical computations. For a factorizing initial condition $\rho(t_0) = \rho_S(t_0) \otimes \rho_B$ we have $\mathscr{P}\rho(t_0) = \rho(t_0)$ and, therefore, $\mathscr{Q}\rho(t_0) = 0$. Hence the inhomogeneous term of the Nakajima-Zwanzig equation 5.4.2.12 vanishes and the exact equation for the relevant part of the density matrix reduces to

$$\frac{\partial \mathscr{P}\rho(t)}{\partial t} = \int_{t_0}^{t} ds \mathscr{K}(t,s)\mathscr{P}\rho(s) \tag{5.4.2.14}$$

To second order in the coupling strength α we obtain

$$\mathscr{K}(t,s) = \alpha^2 \mathscr{P}\mathcal{L}(t)\mathscr{Q}\mathcal{L}(s)\mathscr{P} + \mathcal{O}(\alpha^3) \tag{5.4.2.15}$$

which leads to an equation of motion of second order for $\mathscr{P}\rho(t)$

$$\frac{\partial \mathscr{P}\rho(t)}{\partial t} = \alpha^2 \int_{t_0}^{t} ds \mathscr{P}\mathcal{L}(t)\mathcal{L}(s)\mathscr{P}\rho(s) \tag{5.4.2.16}$$

where we again made use of $\mathscr{P}\mathcal{L}(t)\mathscr{P} = 0$. If we now introduce the explicit expressions for the projection operator $\mathscr{P}$ and for the generator $\mathcal{L}(t)$ we get the Born approximation of the master equation

$$\frac{\partial \rho_S(t)}{\partial t} = -\alpha^2 \int_{t_0}^{t} ds Tr_B[H_I(t), [H_I(s), \rho_S(s) \otimes \rho_B]] \tag{5.4.2.17}$$

which we saw in Eq.5.3.1.7. This approach to the non-Markovian dynamics of open quantum systems has some practical disadvantages. The perturbative approximation of the memory kernel simplifies the derivation of the equations of motion, but unfortunately not their structure. The approximate equation of motion is again an integro-differential equation, whose numerical solution may be quite involved.

5.5 The Quantum Optical Master Equation

In this section, we consider a bound quantum system, e.g. an atom or a molecule, which interacts with a quantized radiation field. The radiation field represents a reservoir with an infinite number of degrees of freedom and the bound system is the reduced system we are interested in. The uncoupled atom or molecule is described by some Hamiltonian H_S, while the free quantized radiation field will be represented by the Hamiltonian (subtracting an infinite c-number for the vacuum energy)

$$H_B = \sum_{\vec{k}} \sum_{\lambda=1,2} \hbar\omega_k b_\lambda^\dagger(\vec{k}) b_\lambda(\vec{k}). \tag{5.5.1}$$

Here, we reintroduce all physical constants such as Planck's constant $\hbar$ and the speed of light c. For simplicity we decompose the radiation field into Fourier modes in a box of volume V, imposing periodic boundary conditions. These modes are labelled by the wave vector $\vec{k}$ and two corresponding, transverse unit polarization vectors $\vec{e}_\lambda(\vec{k})$, such that

$$\vec{k} \cdot \vec{e}_\lambda(\vec{k}) = 0 \tag{5.5.2a}$$

$$\vec{e}_\lambda(\vec{k}) \cdot \vec{e}_{\lambda'}(\vec{k}) = \delta_{\lambda\lambda'} \tag{5.5.2b}$$

$$\sum_{\lambda 1,2} \vec{e}^{\,i}_{\lambda}(\vec{k})\vec{e}^{\,j}_{\lambda} = \delta_{ij} - \frac{k_i k_j}{|\vec{k}|^2}, \quad i,j = 1,2,3 \tag{5.5.2c}$$

The dispersion relation is $\omega_k = ck = c|\vec{k}|$. The field operators $b_\lambda(\vec{k})$ and $b^\dagger_\lambda(\vec{k})$ describe the destruction and creation of photons with wave vector $\vec{k}$ and polarization $\vec{e}_\lambda(\vec{k})$. They obey the commutation relations

$$[b_\lambda(\vec{k}), b_{\lambda'}(\vec{k}')] = [b^\dagger_\lambda(\vec{k}), b^\dagger_{\lambda'}(\vec{k}')] = 0 \tag{5.5.3}$$

$$[b_\lambda(\vec{k}), b_{\lambda'}(\vec{k}')] = \delta\vec{k}\vec{k}'\delta\lambda\lambda'. \tag{5.5.4}$$

Finally, we assume the interaction Hamiltonian to be given in the dipole approximation by

$$H_I = -\vec{D}\cdot\vec{E} \tag{5.5.5}$$

where $\vec{D}$ is the dipole operator of the system under consideration and $\vec{E}$ is the electric field operator in the Schrdinger picture,

$$\vec{E} = i\sum_{\vec{k}}\sum_{\lambda=1,2}\sqrt{\frac{2\pi\hbar\omega_k}{V}}\vec{e}_\lambda(\vec{k})\left(b_\lambda(\vec{k}) - b^\dagger_\lambda(\vec{k})\right). \tag{5.5.6}$$

With these definitions the total Hamiltonian governing the coupled system of the matter degrees of freedom and the radiation degrees of freedom is given by

$$H = H_S + H_B + H_I. \tag{5.5.7}$$

At this point, we performing the Born-Markov approximation. decompose the dipole operator $\vec{D}$ into eigenoperators of H_S. The latter take the form

$$\vec{A}(\omega) \equiv \sum_{\varepsilon' - \varepsilon - \hbar\omega} \Pi(\varepsilon)\vec{D}\Pi(\varepsilon') \tag{5.5.8}$$

Now we have

$$[H_S, \vec{A}(\omega)] = -\hbar\omega\vec{A}(\omega) \tag{5.5.9}$$

$$[H_S, \vec{A}^\dagger(\omega)] = +\hbar\omega\vec{A}^\dagger(\omega) \tag{5.5.10}$$

and

$$\vec{A}^\dagger(\omega) = \vec{A}(-\omega) \tag{5.5.11}$$

The decomposition of the interaction picture dipole operator $\vec{D}(t)$ into eigenoperators therefore reads

$$\vec{D}(t) = \sum_\omega e^{-i\omega t}\vec{A}(\omega) = \sum_\omega e^{+i\omega t}\vec{A}^\dagger(\omega) \tag{5.5.12}$$

and the interaction Hamiltonian can now be written in the interaction picture

$$H_I(t) = -\sum_\omega e^{-\omega t}\vec{A}(\omega)\cdot\vec{E}(t), \tag{5.5.13}$$

where $\vec{E}(t)$ denotes the electric field operator in the interaction picture. Assuming as that

$$\left\langle \vec{E}(t)\right\rangle \equiv Tr\left(\vec{E}(t)\rho_B\right) = 0 \tag{5.5.14}$$

we can immediately write down the equation of motion, analogous to Eq. 5.3.1.21

$$\frac{d\rho_S}{dt} = \sum_{\omega,\omega'} e^{i(\omega'-\omega)t}\Gamma_{ij}(\omega)\left(A_j(\omega)\rho_S A_i^\dagger(\omega') - A_i^\dagger(\omega')A_j(\omega)\rho_S\right) + h.c. \tag{5.5.15}$$

The correlation functions of the electric field operator are defined through

$$\langle E_i(t)E_j(t-s)\rangle \equiv Tr_B\left(E_i(t)E_j(t-s)\rho_B\right) \tag{5.5.16}$$

and their one-sided Fourier transforms are given by

$$\Gamma_{ij}(\omega) \equiv \frac{1}{\hbar^2}\int_0^\infty ds e^{i\omega s}\left\langle E_i(t)E_j(t-s)\right\rangle. \tag{5.5.17}$$

The matrix $\Gamma_{ij}(\omega)$ will be referred to as the spectral correlation tensor. It depends,in general, on t. In fact, without further assumption on the state ρ_B of the reservoir we find

$$\begin{aligned}\Gamma_{ij}(\omega) =& \frac{1}{\hbar^2}\sum_{\vec{k},\vec{k}'}\sum_{\lambda,\lambda'}\sqrt{\frac{2\pi\hbar\omega_k}{V}}\sqrt{\frac{2\pi\hbar\omega_{k'}}{V}}\vec{e}^{\,i}_{\lambda}(\vec{k})\vec{e}^{\,j}_{\lambda'}(\vec{k}') \\ &\times\int_0^\infty ds \Big[\left\langle b_\lambda(\vec{k})b^\dagger_{\lambda'}(\vec{k}')\right\rangle e^{+i(\omega_{k'}-\omega_k)t-i(\omega_{k'}-\omega)s} \\ &+\left\langle b^\dagger_\lambda(\vec{k})b_{\lambda'}(\vec{k}')\right\rangle e^{-i(\omega_{k'}-\omega_k)t-i(\omega_{k'}+\omega)s} \\ &-\left\langle b_\lambda(\vec{k})b^\dagger_{\lambda'}(\vec{k}')\right\rangle e^{-i(\omega_{k'}-\omega_k)t-i(\omega_{k'}+\omega)s} \\ &-\left\langle b^\dagger_\lambda(\vec{k})b_{\lambda'}(\vec{k}')\right\rangle e^{+i(\omega_{k'}-\omega_k)t-i(\omega_{k'}-\omega)s}\Big]\end{aligned} \tag{5.5.18}$$

Chapter 6

Linear Dissipative Dynamics

6.1 Three-Level System (Qutrit)

Three-level systems arise in many physical contexts. A spin-1 particle in an external magnetic field, three states of atoms or molecules coupled by lasers or other interactions, and oscillations among the three neutrino flavours are just a few varied examples. A widely used class of equations, which proceed a full treatment of dissipation and decoherence, is the Liouville von Neumann Lindblad equation [23]

$$
\begin{aligned}
i\hbar\frac{d\rho}{dt} &= [H,\rho] + \frac{1}{2}i\sum_k \Big([L_k\rho, L_k^\dagger] + [L_k, \rho L_k^\dagger]\Big) \\
&= [H,\rho] + \frac{1}{2}i\sum_k \Big(L_k^\dagger L_k\rho + \rho L_k^\dagger L_k - 2L_k\rho L_k^\dagger\Big)
\end{aligned}
\qquad (6.1.1)
$$

where ρ is the density matrix, H is a hermitian Hamiltonian, the L_k are operators in the system through which dissipation and decoherence are introduced. More specifically, the second term on the right-hand side is the Liouvillian super-operator describing coupling to the environment and the resulting irreversibilities of dissipation and decoherence. The above Master Equation 6.1.1 can be expressed in the Liouville - Bloch form as [23]:

$$
i\hbar\frac{d\boldsymbol{\eta}(t)}{dt} = \boldsymbol{\mathcal{L}}(t)\boldsymbol{\eta}(t) \qquad (6.1.2)
$$

where $\boldsymbol{\eta}(t)$ is a column vector whose components $eta_k(t)$, $k = 1, \ldots, n^2 - 1$ are suitable linear combinations of the density matrix elements ,similar to the coherence vector, and $\boldsymbol{\mathcal{L}}$ is a $(n^2-1)\times(n^2-1)$ a matrix which may not be hermitian (from now on $\hbar = 1$) . A convenient choice for eta_k is $\rho_{11} - \rho_{mm}$, $\rho_{nm} + \rho_{mn}$, $\rho_{nm} - \rho_{mn}$ where $m, n = 1, \ldots, n$ and $m > n$. In the case of qubits, $L_k = \sqrt{\frac{\Gamma}{2}}\sigma_k$ $(k = 1, 2, 3)$ and $H = \epsilon(t)\sigma_3 + J\sigma_1$ we have that:

$$
\boldsymbol{\mathcal{L}}(t) = \begin{pmatrix} -i\Gamma & -\epsilon(t) & 0 \\ -\epsilon(t) & -i\Gamma & 2J \\ 0 & 2J & -i\Gamma \end{pmatrix} = -i\Gamma\mathbb{I} - \epsilon(t)A_z + 2JA_x \qquad (6.1.3)
$$

with

$$
A_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad A_y = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad A_z = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (6.1.4)
$$

and $\mathbb{I}$ the 3×3 identity matrix.
Similarly, in the case of qutrits [24], $L_k = \sqrt{\frac{\Gamma}{6}}\lambda_k$ $(k = 1, \ldots, 8)$, and $H = \epsilon(t)A_z + JA_x$ we have that:

$$\begin{aligned}\boldsymbol{\mathcal{L}}(t) &= \begin{pmatrix} -i\Gamma & 0 & 0 & \epsilon(t) & 0 & 0 & 0 & 2J(t) \\ 0 & -i\Gamma & 0 & \sqrt{3}\epsilon(t) & 0 & 0 & 0 & \sqrt{3}2J(t) \\ 0 & 0 & -i\Gamma & 0 & 0 & 2J(t) & 0 & 0 \\ \epsilon(t) & \sqrt{3}\epsilon(t) & 0 & -i\Gamma & 2J(t) & 0 & 0 & 0 \\ 0 & 0 & 0 & 2J(t) & -i\Gamma & 0 & 0 & -\epsilon(t) \\ 0 & 0 & 2J(t) & 0 & 0 & -i\Gamma & -\epsilon(t) & 0 \\ 0 & 0 & 0 & 0 & 0 & -\epsilon(t) & -i\Gamma & 0 \\ 2J(t) & -\sqrt{3}2J(t) & 0 & 0 & -\epsilon(t) & 0 & 0 & -i\Gamma \end{pmatrix} \\ &= -i\Gamma\mathbb{I} + \epsilon(t)B_z + 2J(t)x_x \end{aligned} \tag{6.1.5}$$

where

$$B_x = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\sqrt{3} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad B_y = \begin{pmatrix} 0 & 0 & 0 & 0 & -2i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & i \\ 2i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$B_z = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \end{pmatrix} \tag{6.1.6}$$

and $\mathbb{I}$ the 8×8 identity matrix.
It is clear from Eq. 6.1.3 and 6.1.5 that the form of the matrix $\boldsymbol{\mathcal{L}}(t)$ in qubits and qutrits is common.

CHAPTER 7

APPLIED QUANTUM MASTER EQUATIONS

In this chapter, we will present the master equations that are applied and how do they form in each system under investigation. More analytically, we make use of a Lindblad-type master equation, specially constructed in order to relax to equilibrium (i.e to the Gibbs state and not simply to the fully mixed state) [25]. This is crucial when comparing it to the other master equation that is used, the non-linear thermodynamic quantum master equation, which also relaxes to equilibrium [8].

7.1 Lindblad Master Equation

In this section, we explain how the specific linear markovian master equation in the weak-coupling regime, also known as the Lindblad master equation, is obtained [25]. The constructive approach of Davies [22] is followed, starting from a microscopic point of view.

We consider a quantum system of interest S embedded in a bath B on the Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$. The total Hamiltonian is

$$H = H_S \otimes \mathbb{I} + \mathbb{I} \otimes H_B + \lambda H_I \tag{7.1.1}$$

where H_S is the system Hamiltonian, H_B is the Hamiltonian referring to the bath, H_I is the interaction Hamiltonian and λ is the coupling strength between system and bath (here, is set to 1). The self-adjoint coupling operator Q, acting on the system S, is bound, as is the self-adjoint coupling operator Φ acting on the bath $\mathcal{H}_B$. We have to assume that H_S is bound and has a discrete time-independent N-level spectrum. The dynamics of the system S is then obtained by tracing out the equilibrium bath $\mathcal{H}_B$. The obtained master equation is

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H_S, \rho] + \frac{\lambda^2}{\hbar}\mathcal{K}(\rho) \tag{7.1.2}$$

where ρ is the density matrix, $\mathcal{K}(\rho)$ is the dissipative operator defined on the space of the density matrices and is responsible for the irreversible evolution of the system, λ is the coupling strength between system and bath and $\hbar$ is the reduced Planck or Dirac constant. We here neglect the shift of the free energy levels (it does not affect the final equilibrium solution) and write the dissipative generator as

$$\begin{aligned}\mathcal{K}(\rho) =&\sum_{\omega\geq 0} e(\omega)\left(L_\omega \rho L_\omega^\dagger - \frac{1}{2}\{L_\omega^\dagger L_\omega, \rho\}\right)\\ &+\sum_{\omega\geq 0} \alpha(\omega)\left(L_\omega^\dagger \rho L_\omega - \frac{1}{2}\{L_\omega L_\omega^\dagger, \rho\}\right)\end{aligned} \tag{7.1.3}$$

where the real constant $e(\omega)$ is responsible for the emission processes while $\alpha(\omega)$ is responsible for the absorption processes taking place during the scattering events. The ω's appearing in the sum range in the set of all possible energy transitions of the system, namely, $\omega = Ei - Ej$ for some (i, j) and the sum is taken over all such ω's. The operators L_ω and $L_\omega^\dagger = L_{-\omega}$ are the scattering or Lindblad operators obtained by a spectral decomposition of the self-adjoint coupling operator Q. They model jumps between the eigenstates of the Hamiltonian H_S induced by the scattering of the particles of the system with the particles of the bath. We can see that the Hamiltonian of the system is linked to the Lindblad operators of Eq. 7.1.3 by the relation

$$[L_\omega, H_S] = \omega L_\omega, \tag{7.1.4}$$

which in the energy eigenbasis gives

$$\begin{aligned}\langle E_i \,|\, [L_\omega, H_S] \,|\, E_j\rangle =&(E_j - E_i)\langle E_i \,|\, L_\omega \,|\, E_j\rangle\\ &= (E_j - E_i)(L_\omega)_{ij}\\ &= (E_j - E_i)Q_{ij}\delta_{kr}(E_i - E_j, -\omega),\end{aligned} \tag{7.1.5}$$

where $Q_{ij} = \langle E_i \,|\, Q \,|\, E_j\rangle$ is an ij matrix element of the coupling operator in the energy eigenbasis. The kronecker δ_{kr} in the above equation tells us that only terms with $E_i E_j = \omega$ are non-zero. Moreover, the fact that the Lindblad operators are defined in terms of the energy eigenbasis of the Hamiltonian tells us that when we use a time-dependent Hamiltonian we have to recompute the set of Lindblad operators at each time instant (and possibly obtain a different number of operators due to energy degeneracies or crossings). In practice, one would have to recalculate the Lindblad operator at every integration time step (or at least each time that the spectrum of the Hamiltonian changes).

Concerning the scattering rates, the emission $e(\omega)$ and absorption $\alpha(\omega)$ rates in Eq. 7.1.3 find their origin in the Fourier transformation of the correlation functions of the bath [22]

$$h(t) = \langle \Phi_t \Phi\rangle_B = Tr\left(\rho_B e^{i\frac{H_B}{\hbar}t}\Phi e^{-i\frac{H_B}{\hbar}t}\right) \tag{7.1.6}$$

where $\rho_B = \frac{e^{-\beta H_B}}{Z_B}$ is the Gibbs state of the bath, $Z_B = Tr(e^{-\beta H_B})$ and $\beta = \frac{1}{k_B T}$ is the fixed inverse temperature of the bath. The emission and absorption spectral functions exist if $\int_0^t |h(t)| < 0$, in which case we find that

$$\hat{h}(\omega) = \frac{1}{\hbar}\int_{-\infty}^{+\infty} e^{i\omega t} h(t)dt, \tag{7.1.7}$$

$$\hat{h}(\omega) = e(\omega), \quad \omega \geq 0, \hat{h}(\omega) = a(\omega), \quad \omega < 0. \tag{7.1.8}$$

During the time evolution, a given energy level will gain and loose excitations. More precisely, the terms $L_\omega \rho L_\omega^\dagger$ and $L_\omega^\dagger \rho L_\omega$ are responsible for the gain while the terms $\{L_\omega^\dagger \rho L_\omega\}$ and $\{L_\omega \rho L_\omega^\dagger\}$ are responsible for the loss. Therefore, to reach equilibrium, it is necessary to have a proper detailed balance among the emissions and the absorptions. Hence, having

$$\alpha(\omega) = e^{-\beta\omega} e(\omega), \tag{7.1.9}$$

insures that the master equation converges to an equilibrium state [22] by balancing the incoming and outgoing scattering for standard ergodic conditions (every energy level should be connected to the others, at least indirectly). The precise form of the emission $e(\omega)$ and absorption $\alpha(\omega)$ rate present in the master equation given by 7.1.3 depend on the nature of the bath (bosonic, fermionic, anionic, etc.).

7.1.1 Three-Level System (Qutrit)

The first system under investigation is the three-level, often named qutrit. For such a system with non-degenerated energy levels, we have seven Lindblad operators. More precisely,

$$\begin{gathered}
\boldsymbol{L}_{12} = \begin{pmatrix} 0 & Q^{12} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{L}_{21} = \begin{pmatrix} 0 & 0 & 0 \\ Q^{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\boldsymbol{L}_{13} = \begin{pmatrix} 0 & 0 & Q^{13} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{L}_{31} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ Q^{31} & 0 & 0 \end{pmatrix}, \\
\boldsymbol{L}_{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & Q^{23} \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{L}_{32} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & Q^{32} & 0 \end{pmatrix}, \\
\boldsymbol{L}_{11} = \begin{pmatrix} Q^{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{L}_{22} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & Q^{22} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{L}_{33} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & Q^{33} \end{pmatrix}.
\end{gathered} \tag{7.1.1.1}$$

where Q^{ij} $(i,j = 1,2,3)$ are the (i,j) element of matrix $\boldsymbol{Q}$ defined later.

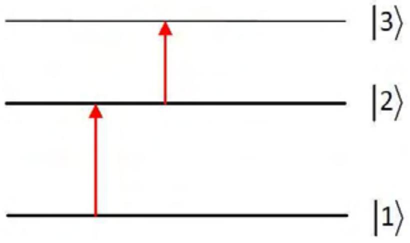


Figure 7.1.1: A three-level system (qutrit) with basis states $|1\rangle$, $|2\rangle$ and $|3\rangle$

We can rewrite these matrices in the form

$$\boldsymbol{L}_{ij} = Q^{ij} \boldsymbol{\sigma}^{ij}, \tag{7.1.1.2}$$

with $Q^{ij} = Q^{ji*}$ and by defining the 3×3 σ_{ij} basis matrices as follows,

$$\boldsymbol{\sigma}_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{\sigma}_{21} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_{32} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_{31} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{7.1.1.3}$$

$$\boldsymbol{\sigma}_{11} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_{22} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_{33} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with $\boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ji}^{\dagger}$. The resulting dissipative operator, Eq. 7.1.3, is of the form

$$\begin{aligned} \mathcal{K}^{TL}(\rho) = & \sum_{\omega_{ij,k}} \Bigg[\Gamma^{ij}_{em,k} \left(\boldsymbol{\sigma}_{ij} \rho \boldsymbol{\sigma}^{\dagger}_{ij} - \frac{1}{2} \left\{ \boldsymbol{\sigma}^{\dagger}_{ij} \boldsymbol{\sigma}_{ij}, \rho \right\} \right) \\ & + \Gamma^{ji}_{ab,k} \left(\boldsymbol{\sigma}^{\dagger}_{ij} \rho \boldsymbol{\sigma}_{ij} - \frac{1}{2} \left\{ \boldsymbol{\sigma}_{ij} \boldsymbol{\sigma}^{\dagger}_{ij}, \rho \right\} \right) \Bigg] \\ & + \sum_{\omega_{ii}} \Gamma^{ii}_{dp,k} \left(\boldsymbol{\sigma}_{ii} \rho \boldsymbol{\sigma}_{ii} - \frac{1}{2} \left\{ \boldsymbol{\sigma}_{ii} \boldsymbol{\sigma}_{ii}, \rho \right\} \right) \end{aligned} \tag{7.1.1.4}$$

where we used the fact that $\boldsymbol{\sigma}_{ii}\boldsymbol{\sigma}_{jj} = 0$ for $i \neq j$ (this eliminates the cross terms in the dephasing terms). Moreover, we can simplify the equation with the general properties $\boldsymbol{\sigma}_{ij}\boldsymbol{\sigma}_{ji} = \boldsymbol{\sigma}_{ii}$ and $\boldsymbol{\sigma}_{ji}\boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{jj}$. Also, $\Gamma^{ij}_{em,k}$, $\Gamma^{ij}_{ab,k}$ and $\Gamma^{ii}_{dp,k}$, with $k = l, r$ (l:left, r:right heat bath) and $i, j = 1, 2, 3$ $(j > i)$, are scattering rates referring to emission, absorption and dephasing respectively, given by Eq. 7.1.1.5,7.1.1.6 and 7.1.1.7 below,

$$\Gamma^{ij}_{em,k} = e_k(\omega_{ij}) \left| \tilde{Q}^{ji,k} \right|^2 = e^{\beta_k \omega^{ij}} \frac{2\gamma_k}{\beta_k} \left| \tilde{Q}^{ji,k} \right|^2 \tag{7.1.1.5}$$

$$\Gamma^{ij}_{ab,k} = \alpha_k(\omega_{ij}) \left| \tilde{Q}^{ji,k} \right|^2 = \frac{2\gamma_k}{\beta_k} \left| \tilde{Q}^{ji,k} \right|^2 \tag{7.1.1.6}$$

$$\Gamma^{ii}_{dp,k} = e_k(0) \left| \tilde{Q}^{ii,k} \right|^2 = \frac{2\gamma_k}{\beta_k} \left| \tilde{Q}^{ii,k} \right|^2 \tag{7.1.1.7}$$

where $\omega_{ij} = \{\omega_{12}, \omega_{23}, \omega_{13}\}$, $\omega_{ii} = \{\omega_{11}, \omega_{22}, \omega_{33}\}$ and $\beta_k = \frac{1}{k_B T_k}$. To reach equilibrium, it is necessary to have a proper detailed balance among the emissions and absorptions, Eq. 7.1.9. The choice for $\alpha_k(\omega_{ij})$ and $e_k(\omega_{ij})$ can be done using a "flat" spectrum, independent of the frequency,

$$\alpha_k(\omega_{ij}) = \frac{2\gamma_k}{\beta_k} \tag{7.1.1.8}$$

where γ is the friction, to be as close as possible to the non-linear master equation. Now, from Eq.7.1.9 we get the following

$$e_k(\omega_{ij}) = \frac{2\gamma_k}{\beta_k} e^{\beta_k \omega_{ij}} \tag{7.1.1.9}$$

The Hamiltonian in the case of the three-level system (qutrit) is of the form

$$H_S = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} \tag{7.1.1.10}$$

where

$$E_j = \hbar\omega_{ij} + E_i \tag{7.1.1.11}$$

is the energy of each state ($i = 1, 2, 3$) and ω_{ig} are the eigenfrequencies.

7.1.2 Harmonic Oscillator (10 states)

In the case of the harmonic oscillator with 10 states, the distance among the energy levels is equal,

$$E_n = n + \frac{1}{2}, n = 0, \ldots, 9 \tag{7.1.2.1}$$

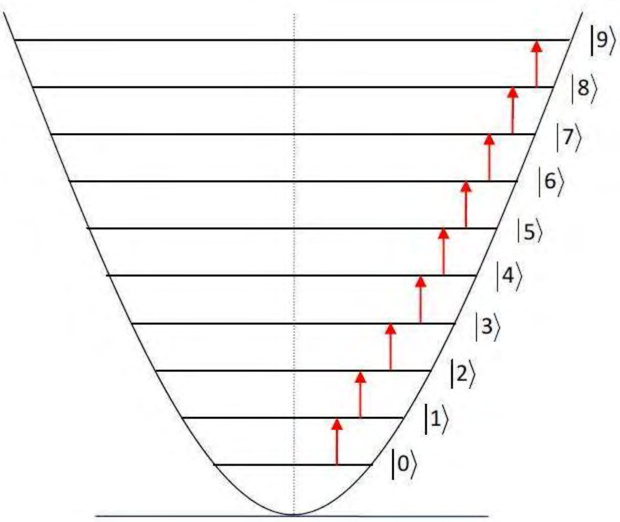


Figure 7.1.2.1: The quantum harmonic oscillator system (10 states) with basis states $|0\rangle$, $\ldots$, $|9\rangle$

Subsequently, the value of $\omega_{i,i+1}$ is the same among the energy levels of the system. In this case of degenerated energy levels, we have less Lindblad operators. More precisely, we get the following three Lindblad operators

- L_{em}, which corresponds to the emission terms ($\omega_{ij} = \omega$)
- L_{ab}, which corresponds to the absorption terms ($\omega_{ji} = -\omega$)
- L_{dp}, which corresponds to the dephasing terms ($\omega_{ii} = \omega_0$)

The dissipative operator, Eq. 7.1.2, now takes the form

$$\begin{aligned} K^{HO}(\rho) = \sum_{k=l,r} \Bigg[& \Gamma_{em,k} \left(L_{em,k}\rho L^{\dagger}_{em,k} - \frac{1}{2}\left\{ L^{\dagger}_{em,k} L_{em,k}, \rho \right\} \right) \\ & + \Gamma_{ab,k} \left(L^{\dagger}_{ab,k}\rho L_{ab,k} - \frac{1}{2}\left\{ L_{ab,k} L^{\dagger}_{ab,k}, \rho \right\} \right) \\ & + \Gamma_{dp,k} \left(L_{dp,k}\rho L_{dp,k} - \frac{1}{2}\left\{ L_{dp,k} L_{dp,k}, \rho \right\} \right) \Bigg] \end{aligned} \tag{7.1.2.2}$$

with

$$\boldsymbol{L}_{em,k} = \sum_{i=1}^{9} Q^{ii+1,k} \boldsymbol{\sigma}_{ii+1} \tag{7.1.2.3}$$

$$\boldsymbol{L}_{ab,k} = \sum_{i=2}^{10} Q^{ii-1,k} \boldsymbol{\sigma}_{ii-1} \tag{7.1.2.4}$$

$$\boldsymbol{L}_{dp,k} = \sum_{i=1}^{10} Q^{ii,k} \boldsymbol{\sigma}_{ii} \tag{7.1.2.5}$$

Now, $\boldsymbol{\sigma}_{ij}$ are 10×10, zero-valued matrices, with the corresponding ij element being the only non-zero (similar to Eq. 7.1.1.3). The system Hamiltonian is the following 10×10 matrix

$$H_S = \begin{pmatrix} E_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_9 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_{10} \end{pmatrix} \tag{7.1.2.6}$$

where

$$E_j = \hbar\omega_{ij} + E_i \tag{7.1.2.7}$$

is the energy of each state ($i = 1, .., 10$) and ω_{ig} are the eigenfrequencies.

7.2 Thermodynamic Quantum Master Equation

7.2.1 Classical Environment

The approach that we use in order to describe dissipative quantum systems is carefully motivated by [10] and is intended to describe the dynamics of a quantum subsystem coupled to an arbitrary, possibly time-dependent environment. For that purpose, we need a powerful formalism to describe the classical environmental degrees of freedom and is succeeded The choice that as been made in [8], [12], [10] relies on an extension of the GENERIC building block of classical nonequilibrium systems [11]. But before we go on, we will try to briefly present the basic features of this powerful formalism.

7.2.2 GENERIC

In non-equilibrium thermodynamics, GENERIC is an acronym for **G**eneral **E**quation for **N**on-**E**quilibrium **R**eversible-**I**rreversible **C**oupling. It is the general form of dynamic equation for a system with both reversible and irreversible dynamics (generated by energy and entropy, respectively). GENERIC formalism is the theory built around the GENERIC equation, which has been proposed in its final form in 1997 by Miroslav Grmela and Hans Christian Öttinger [26], [27].

The GENERIC equation is the following

$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E}{\delta x}(x) + M(x) \cdot \frac{\delta S}{\delta x}(x) \tag{7.2.2.1}$$

where x denotes the set of independent variables required for a complete description of the non-equilibrium system, $E(x)$ and $S(x)$ are the system's total energy and entropy expressed in terms of the state variables x, and $L(x)$ and $M(x)$ are certain linear operators (or matrices). Since x typically contains position dependent fields, such as mass, momentum, and energy densities, the state variables are usually labelled by continuous (position) labels in addition to discrete ones. A matrix multiplication, or the application of a linear operator, hence implies not only summations over discrete labels but also integrations over continuous labels and $\frac{\delta}{\delta x}$ typically implies functional rather than partial derivatives. More specifically, $L(x)$ is the Poisson matrix and is an antisymmetric matrix describing the reversible dynamics of the system according to Hamiltonian mechanics. $M(x)$ is the friction matrix and is a positive semidefinite (and hence symmetric) matrix describing the systems irreversible behaviour.

In addition to the above equation and the properties of its constituents, systems that ought to be properly described by the GENERIC formalism are required to fulfil the following degeneracy conditions

$$L(x) \cdot \frac{\delta S}{\delta x}(x) = 0 \tag{7.2.2.2}$$

which express the conservation of entropy under reversible dynamics (the functional form of the entropy is such that it cannot be affected by the operator generating the reversible dynamics), and

$$M(x) \cdot \frac{\delta E}{\delta x}(x) = 0 \tag{7.2.2.3}$$

which express the conservation of energy under irreversible dynamics.

Further general properties of L and M are discussed most conveniently in terms of the two brackets

$$\{A, B\} = \frac{\delta A}{\delta x} L(x) \frac{\delta B}{\delta x} \tag{7.2.2.4a}$$

which is the Poisson bracket, and

$$[A, B] = \frac{\delta A}{\delta x} M(x) \frac{\delta B}{\delta x} \tag{7.2.2.4b}$$

which is the dissipative bracket, where A and B are sufficiently regular real-valued functions on the state space. The Poisson bracket, Eq. 7.2.2.4a, has the following properties:

a It is bilinear

b $\{A, B\} = -\{B, A\}$, stated as the antisymmetry property,

c $\{A, B, C\} = A\{B, C\} + B\{A, C\}$

d $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, CB\}\} = 0$, known as the Jacobi identity and which express the time invariance of the Poisson bracket,

where C is an arbitrary sufficiently regular real-valued function on the state space. The dissipative bracket, 7.2.2.4b, has the following properties:

a It is bilinear

b $[A, B] = [B, A]$, stated as the symmetry property,

c $[A, A] \geq 0, \forall A$, stated as the non-negativeness condition.

From 7.2.2.2 (implying S,E = 0) and the non-negativeness condition above, guarantees that the entropy is a non-decreasing function of time

$$\frac{dS}{dt} \geq 0. \tag{7.2.2.5}$$

In terms of these brackets, 7.2.2.1, 7.2.2.4a and 7.2.2.4b and the chain rule lead to the following time-evolution equation of an arbitrary function A in terms of the two separate generators E and S:

$$\frac{dA}{dt} = \{A, E\} + [A, S] \tag{7.2.2.6}$$

where the first right-side term refers to reversible dynamics, whereas the second right-hand side term refers to irreversible dynamics. A similar equation already existed from A. N. Beris & B.J. Edwards [28]

$$\frac{dA}{dt} = \{A, F\} + [A, F] \tag{7.2.2.7}$$

where $F = E - TS$ is the free energy and is recognized also as a special case of the GENERIC approach [27].

The proper arena for quantum mechanics is provided by separable complete Hilbert spaces, that is, complex vector spaces equipped with inner products. Observables are densely defined self-adjoint linear operators on a Hilbert space $\mathcal{H}$. As a consequence of self-adjointness, observables are real. For nonequilibrium systems, we are interested in the evolution of the averages of a sufficiently rich set of observables. It is not immediately obvious what sufficiently rich means for the characterization of the state of a quantum system. We here focus on the evolution of the density matrix ρ, also known as the statistical operator, which can be expressed in terms of an orthonormal basis $|n\rangle$ of the Hilbert space $\mathcal{H}$ and the probabilities p_n, namely,

$$\rho = \sum_n p_n |n\rangle \langle n| \,. \tag{7.2.2.8}$$

The density matrix characterizes the state of our quantum subsystem and its time evolution determines the evolution of the averages of all observables.

The corresponding arena for classical systems is given by functions or functionals on a Poisson manifold as observables. Classical nonequilibrium thermodynamics provides evolution equations for the values of observables in terms of Poisson and dissipative brackets as the appropriate geometric structures [11], [28], [26], [27]. In practice, one usually follows the evolution of a point x in a Poisson manifold. The evaluation of observables as functions or functionals of the state variable(s) x is the classical counterpart of the averaging of quantum observables with a density matrix ρ.

The key idea is the need for separate geometric structures for generating reversible and irreversible dynamics from energy and entropy, respectively. In quantum mechanics, the Hamiltonian and von Neumann's entropy are available. The proper structure underlying reversible mechanics is known to be given by the quantum Poisson bracket of two observables A and B in terms of their commutator and Planck's constant $\hbar$,

$$(A, B) = \frac{1}{i\hbar}[A, B] \tag{7.2.2.9}$$

motivated and introduced by Dirac [17]. The symbol (A, B) is used for the quantum Poisson bracket and it should not be confused with the scalar product. The rate of reversible change of the average $\langle A\rangle_\rho = Tr(A\rho)$ of a quantum observable A is given by the average $\langle (A, H)\rangle_\rho$, where the observable H is the Hamiltonian of the quantum system. In the same spirit, we next propose the simple geometric structure behind all irreversible dynamics. The essential structural element is $\langle (A, Q); (B, Q)\rangle_\rho$ where Q is an operator that provides the weak dissipative coupling of the quantum subsystem with its environment. The bilinear pairing $\langle ; \rangle_\rho$ in its structural element is the canonical correlation [29]

$$\langle A; B\rangle_\rho = \int_0^1 Tr(\rho^\lambda A \rho^{1-\lambda} B) d\lambda = Tr(A_\rho B), \tag{7.2.2.10}$$

where

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda, \tag{7.2.2.11}$$

is basically the product of the observable A and the density matrix ρ but, it's necessary to compromise between writing ρ to the left or the right of A, it is placed as a subscript. The canonical correlation has the following properties:

a. it is symmetric,

$$\langle A; B\rangle_\rho = \langle B; A\rangle_\rho \tag{7.2.2.12}$$

for all observables A, B, and

b. It is positive,

$$\langle A; A\rangle_\rho \geq 0, \tag{7.2.2.13}$$

for all observables A.

Additional properties can be inferred from Lieb's theorem [2]

$$f_t(A, B) = -Tr\{X^+ A^t X B^{1-t}\} \tag{7.2.2.14}$$

The functional f_t is jointly convex in its arguments A and B, where A, B are positive operators, X is an arbitrary fixed operator and t is a fixed number in the interval $[0, 1]$. In the very same way that the reversible structure $\langle (A, B)\rangle_\rho$ assists the Hamiltonian to generate reversible evolution, irreversible evolution should be generated by entropy by means of the irreversible geometric structure $\langle (A, Q); (B, Q)\rangle_\rho$. Assuming von Neumann's logarithmic form of the entropy, this possibility relies on the following identity:

$$(ln\rho, A_\rho) = (\rho, A). \tag{7.2.2.15}$$

To prove this result, which is crucial for a thermodynamically consistent construction of irreversible dynamics generated by von Neumanns entropy, we can look at arbitrary matrix elements formed with the eigenstates of the density matrix

$$\begin{aligned}(lnp_n - lnp_m)\, \langle n \,|\, A_{rho} \,|\, m\rangle &= p_m ln\frac{p_n}{p_m} \int\limits_0^1 \left(\frac{p_n}{p_m}^\lambda\right) d\lambda\, \langle n \,|\, A \,|\, m\rangle \\ &= (p_n - p_m)\, \langle n \,|\, A \,|\, m\rangle\,.\end{aligned} \tag{7.2.2.16}$$

At this point, all the essential ingredients of nonequilibrium thermodynamics have been presented and the formulation of the general evolution equations for dissipative quantum systems is straightforward. The only new element is the canonical correlation of two commutators required to construct irreversible dynamics from the entropy.

In order to obtain the total energy and entropy of a closed system consisting of a quantum subsystem and its classical environment it is necessary to know the corresponding pairs $\tilde{A}$ of quantum and classical observables, A and A_e, so that on can write

$$\tilde{A} = \langle A\rangle_\rho + A_{e,x}. \tag{7.2.2.17}$$

where the subscript x indicates that an observable is evaluated in the classical state x. For the energy $\tilde{H}$, A is the Hamiltonian H of the quantum subsystem and A_e is the energy H_e of the environment. For the entropy $\tilde{S}$, the following $S = -k_B ln\rho$ is chosen as operator A, where k_B is the Boltzmann's constant, and A_e is the entropy S_e of the classical environment. Then, the evolution of the average $\bar{A}$ of any joint observable $\tilde{A}$ of the quantum system and its environment can be formulated in terms of the generators $\tilde{H}$ and $\tilde{S}$,

$$\frac{\tilde{A}}{dt} = \mathcal{P}(\tilde{A}, \tilde{H}) + \mathcal{D}(\tilde{A}, \tilde{S}), \tag{7.2.2.18}$$

where $\mathcal{P}$ is the reversible Poisson contribution, while $\mathcal{D}$ is the irreversible dissipative contribution. Both contributions consist of classical and quantum-mechanical contributions. This formulation is the most natural generalization of the GENERIC framework of classical nonequilibrium thermodynamics [11], [26], [27]. So,

$$\mathcal{P}(\tilde{A}, \tilde{B}) = \boldsymbol{\{}A_e, B_e\boldsymbol{\}}_x + \langle (A, B)\rangle_\rho\,, \tag{7.2.2.19}$$

where $\boldsymbol{\{},\boldsymbol{\}}$ is the classical Poisson bracket and it should not be confused with the anticommutator in quantum mechanics. The distinction between classical Poisson brackets and quantum anticommutators (both expressed as curly brackets) as well as between classical dissipative brackets and quantum commutators (both expressed as square brackets) should always be clear from the context, and this distinction is facilitated by using boldface brackets for the classical objects. For the dissipative contribution to evolution we employ the following bracket structure:

$$\begin{aligned}\mathcal{D}(\tilde{A},\tilde{B}) =&[A_e,B_e]_x + [H_e,H_e]^Q_x\langle(A,Q);(B,Q)\rangle_\rho\\ &-[A_e,H_e]^Q_x(H,Q);(B,Q)\rangle_\rho\\ &-[H_e,B_e]^Q_x(A,Q);(H,Q)\rangle_\rho\\ &+[A_e,B_e]^Q_x(H,Q);(H,Q)\rangle_\rho\end{aligned} \tag{7.2.2.20}$$

The standard classical dissipative bracket, $[,]$, and the dissipative bracket, $[,]^Q$, are both symmetric and positive semidefinite, but the latter does not need to fulfill the usual GENERIC degeneracy expressing energy conservation. This conservation of energy is guaranteed by the form of 7.2.2.20, which is actually motivated by energy conservation and that is why the last three compensation terms are needed. All the essence of the dissipative bracket is contained in the first line of Eq. 7.2.2.20. As the coupling between the quantum system and its classical environment is purely irreversible, the entropy of each subsystem is conserved by its own reversible dynamics, $\boldsymbol{\{}A_e,S_e\boldsymbol{\}}=0$ and $\langle(A,S)\rangle_\rho = 0$ for arbitrary observables A_e and A. The dissipative structure, Eq. 7.2.2.20 can be generalized by summing up contributions from several different coupling operators Q, each of them coming with its own classical dissipative bracket $[,]^Q$. Also, The different irreversible processes could even be coupled.

Considering now the fundamental equation 7.2.2.18 along with the reversible and irreversible contributions, Eqs 7.2.2.19 and 7.2.2.20 respectively, and separating the contributions involving the quantum observable A and the classical observable A_e, the following equation is obtained for the evolution of averages in the quantum subsystem:

$$\begin{aligned}\frac{d\langle A\rangle_\rho}{dt} = \langle(A,H)\rangle_\rho - [H_e,S_e]^Q_x\,\langle(A,Q);(H,Q)\rangle_\rho&\\ +k_B[H_e,H_e]^Q_x\,\langle(Q,(Q,A))\rangle_\rho\,.&\end{aligned} \tag{7.2.2.21}$$

The classical environment is governed by the evolution equation

$$\begin{aligned}\frac{dA_{e,x}}{dt} =&\boldsymbol{\{}A_e,H_e\boldsymbol{\}}_x - k_B[A_e,H_e]^Q_x\,\langle(Q,(Q,H))\rangle_\rho\\ &+[A_e,S_e]_x + [A_e,S_e]^Q_x\,\langle((H,Q);(H,Q))\rangle_\rho\,.\end{aligned} \tag{7.2.2.22}$$

From the consistent evolution of the averages of arbitrary observables A one can infer the underlying evolution equation for the density matrix ρ. Indeed, the following master equation for the density matrix reproduces the evolution equation 7.2.2.21 for arbitrary averages

$$\begin{aligned}\frac{d\rho}{dt} =&-(\rho,H) + [H_e,S_e]^Q_x(Q,(Q,H)_\rho)\\ &+k_B[H_e,H_e]^Q_x(Q,(Q,\rho))\end{aligned} \tag{7.2.2.23}$$

as can be verified by means of the identities

$$\langle (A,H)\rangle_\rho = -Tr[A(\rho,H)] \tag{7.2.2.24}$$

$$\langle (Q,(Q,A))\rangle_\rho = Tr[A(Q,(Q,\rho))] \tag{7.2.2.25}$$

$$\langle (A,Q);(H,Q)\rangle_\rho = -Tr[A(Q,(Q,H)_\rho)] \tag{7.2.2.26}$$

$$\langle A\rangle_\rho = Tr(A\rho) \tag{7.2.2.27}$$

which follow directly from the definitions 7.2.2.9 and 7.2.2.10. The master equation 7.2.2.23 is our fundamental equation for open quantum systems. The existence of a master equation implies that the evolution of all averages is formulated in a consistent way. In view of the definition 7.2.2.11, the second term in Eq. 7.2.2.23 will, in general, be nonlinear in ρ. This quantum nonlinearity of an irreversible contribution caused by noncommutativity of observables implies that the above master equation cannot be of the popular Lindblad form [9]. The most natural linear approximation to the GENERIC master equation 7.2.2.23 is obtained in terms of the symmetric anticommutator

$$(Q,H)_\rho \approx \frac{1}{2}\{(Q,H),\rho\}, \tag{7.2.2.28}$$

possibly in combination with a modification of the coefficients. Note, however, that linearizations spoil the thermodynamic structure and are hence not recommendable. In particular, the nonlinearity guarantees a proper equilibrium solution.

A similar master equation of the form of 7.2.2.23, referring to an arbitrary quantum system in contact with a heat bath, has been derived from H. Grabert in 1982 [5] by projection operator techniques with a relevant ensemble of the exponential form, given in the next section.

7.2.3 Derivation by Projection Operator Techniques

As a general example of the GENERIC master equation 7.2.2.23 is provided by an arbitrary quantum system in contact with a heat bath, for which H. Grabert [5] has derived a quantum master equation by projection operator techniques with a relevant ensemble of the exponential form. That derivation was motivated by the failure of the frequently used quantum regression hypothesis, which assumes that the decay of two-time correlations is governed by exactly the same evolution equation as the decay of averages and which is an essential part of the linear standard theory of quantum Markov processes.

To begin with, the Hilbert space $\mathcal{H}$ of the entire system is the tensor product of the Hilbert spaces of $\mathcal{H}_S$ and $\mathcal{H}_R$ of the two subsystems S and R. The trace Tr over a complete set of orthnomal functions in $\mathcal{H}$ can be carried out in two steps

$$Tr = tr tr_R \tag{7.2.3.1}$$

where tr and tr_R denote the partial traces over a complete set of orthonormal states in $\mathcal{H}_S$ and $\mathcal{H}_R$, respectively. The state of the subsystem S is described by the reduced density matrix

$$\rho(t) = Tr_R = W(t) \tag{7.2.3.2}$$

where $W(t)$ is the density matrix of the entire system. Because of Eq. 7.2.3.1, the mean value of any variable u of S is found to be

$$\langle u(t)\rangle = Tr(uW(t)) = tr(u\rho(t)) \tag{7.2.3.3}$$

so that $\rho(t)$ contains complete information about S. In thermal equilibrium the state of $S \otimes R$ is described by a canonical density matrix

$$W_\beta = Z_\beta^{-1} e^{-\beta \mathscr{H}}, \quad Z_\beta = Tr(e^{-\beta \mathscr{H}}) \tag{7.2.3.4}$$

where $\mathscr{H}$ is the Hamiltonian of the entire system. The corresponding reduced matrix reads

$$\rho_\beta = tr_R W_\beta. \tag{7.2.3.5}$$

On defining an effective Hamiltonian H of S vy

$$H = \frac{1}{\beta} ln tr_R e^{-\beta(H)}, \tag{7.2.3.6}$$

the equilibrium state of S may be written as

$$\rho_\beta = Z_\beta^{-1} e^{-\beta H}. \tag{7.2.3.7}$$

Since H will depend on the reservoir temperature in general, it might more appropriately be called the free energy operator of S. We now consider a nonequilibrium state. Given the reduced density matrix $\rho(t)$ of S, we may introduce a relevant density matrix $\bar{W}(t)$ of $S \otimes R$ by

$$\bar{W}(t) = Z(t)^{-1} e^{-\beta(\mathscr{H} - \mu(t))}, \quad Z(t) = Tr(e^{-\beta(\mathscr{H} - \mu(t))}) \tag{7.2.3.8}$$

where $\mu(t)$ is an operator acting in the Hilbert space H_S of S only. This operator is determined by the requirement

$$tr_R \bar{W}(t) = \rho(t). \tag{7.2.3.9}$$

Hence, as far as the state of the subsystem S is concerned, the relevant density matrix $\bar{W}(t)$ and the true density matrix $W(t)$ are equivalent. Furthermore, an initial nonequilibrium state prepared by applying a perturbation H_ext to the subsystem S is of the form 7.2.3.8 with $\mu(t) = -H_{ext}$. $\mu(t)$ may be looked upon as a thermodynamic force operator conjugate to the reduced density matrix $\rho(t)$. A small change $\delta\mu(t)$, of this force operator leads to a change $\delta\bar{W}(t)$ of the relevant density matrix 7.2.3.8 given by

$$\delta \bar{W}(t) = \beta \mathscr{K}(t)(\delta\mu(t) - \langle \delta\bar{\mu(t)} \rangle) \tag{7.2.3.10}$$

where

$$\mathscr{K}(t)U = (Z(t)\beta)^{-1} \int_0^\beta d\alpha e^{-\alpha(\mathscr{H} - \mu(t))} U e^{-(\beta-\alpha)(\mathscr{H} - \mu(t))} \tag{7.2.3.11}$$

and

$$\langle \delta\bar{\mu(t)} \rangle = Tr(\delta\mu(t)\bar{W}(t)). \tag{7.2.3.12}$$

Since a change of $\mu(t)$ by a c-number has no effect on $\bar{W}(t)$ but is cancelled by the associated change of the normalization factor $Z(t)$, without a loss of generality it may assumed

$$\langle \delta\bar{\mu(t)} \rangle = 0. \tag{7.2.3.13}$$

From Eqs 7.2.3.8 and7.2.3.10 it is obtained for the change $\delta\rho(t)$ of the reduced density matrix

$$\delta\rho = \beta \boldsymbol{k}(t)\delta\mu(t) \tag{7.2.3.14}$$

where

$$\begin{aligned}\boldsymbol{k}(t)u &= Tr_R(\mathscr{K}(t)u)\\ &= (Z(t)\beta)^{-1}\int\limits_0^{\beta} d\alpha tr_R(e^{-\alpha}(\mathscr{H}-\mu(t))ue^{-(\beta-\alpha)(\mathscr{H})-\mu(t)}).\end{aligned} \tag{7.2.3.15}$$

$\mathscr{K}(t)$ is a super-operator defined as a transformation of operators U of the entire system $S\otimes R$, while $\boldsymbol{k(t)}$ is defined as a transformation of operators u of the subsystem S. At this point, it is necessary to distinguish $\boldsymbol{k}(t)$ and $Tr_R(\mathscr{K}(t))$ in general. The transformation $tr_R(\mathscr{K}(t))$ reduces operators acting in $\mathcal{H}$ to operators acting in $\mathcal{H}_S$ only. However, the two transformations $\boldsymbol{k(t)}$ and $Tr_R(\mathscr{K}(t))$ coincide when they are applied to the subsystem S. Through combination of Eqs 7.2.3.2, 7.2.3.10, 7.2.3.13, 7.2.3.14 it is found that

$$\delta\bar{W}(t) = \mathscr{P}(t)\delta W(t) \tag{7.2.3.16}$$

where

$$\mathscr{P}(t) = (K)(t)\boldsymbol{k}(t)^{-1}tr_R \tag{7.2.3.17}$$

is a projection operator. From Eqs 7.2.3.15 and 7.2.3.16 we see that this projection operator has the following properties

$$\mathscr{P}(t)\mathscr{P}({}'t) = \mathscr{P}(t) \tag{7.2.3.18a}$$

and

$$\dot{\bar{W}}(t) = \mathscr{P}(t)\dot{W}(t). \tag{7.2.3.18b}$$

The true density matrix $W(t)$ obeys the Liouville - von Neumann equation

$$\dot{W}(t) = -i\mathscr{L}(t)W(t). \tag{7.2.3.19}$$

The Liouville operator $\mathscr{L}(t)$ of the entire system $S\otimes R$ may contain a time-dependent part of due to an external perturbation $H_{ext}(t)$ acting upon S

$$\mathscr{L}(t) = \frac{1}{\hbar}[\mathscr{H}+H_{ext},\%]. \tag{7.2.3.20}$$

By decomposing $W(t)$ into

$$W(t) = \bar{W}(t) + \Delta W(t) \tag{7.2.3.21}$$

where $\Delta W(t)$ is the deviation from the relevant form, from Eqs 7.2.3.18b 7.2.3.19 they are obtained two coupled equations of motions

$$\dot{\bar{W}}(t) = -i\mathscr{P}(t)\mathscr{L}(t)\bar{W}(t) - i\mathscr{P}(t)\mathscr{L}(t)\Delta W(t) \tag{7.2.3.22}$$

and

$$\Delta\dot{W}(t) = -i(1-\mathscr{P}(t))\mathscr{L}(t)\bar{W}(t) - i(1-\mathscr{P}(t))\mathscr{L}(t)\Delta W(t). \tag{7.2.3.23}$$

The integration of 7.2.3.23 leads to

$$\Delta W(t) = \mathscr{G}(t,0)\Delta W(0) - \int\limits_0^t ds\mathscr{G}(t,s)(1-\mathscr{P}(s))i\mathscr{L}(s)\bar{W}(s). \tag{7.2.3.24}$$

Here we have introduced the time-ordered exponential

$$\mathscr{G}(t,s) = Te^{-\int_{s}^{(1-\mathscr{P}(u))i\mathscr{L}(u)} du()} \tag{7.2.3.25}$$

where operators are ordered from right to left as time increases. Inserting 7.2.3.24 into 7.2.3.22, it is found that

$$\dot{\bar{W}}(t) = -i\mathscr{P}(t)\mathscr{L}(t)\bar{W}(t) - \int_0^t ds\mathscr{P}(t)\mathscr{L}(t)\mathscr{G}(t,s)(1-\mathscr{P}(s))\mathscr{L}(s)\bar{W}(s) - i\mathscr{P}(t)\mathscr{L}(t)\mathscr{G}(t,0)\Delta W(0). \tag{7.2.3.26}$$

We will assume that the initial nonequilibrium state has been prepared by means of a constant external perturbation applied to the subsystem S. When at time $t = 0$ the steady state in the presence of this perturbation has been reached, the initial nonequilibrium density matrix $W(0)$ is of the relevant form. Then

$$\Delta W(0) = 0, \tag{7.2.3.27}$$

and the last term in Eq. 7.2.3.26 vanishes. From Eq. 7.2.3.15 and 7.2.3.17 we get

$$tr_R\mathscr{P}(t) = tr_R. \tag{7.2.3.28}$$

Using 7.2.3.9, 7.2.3.27, 7.2.3.28 it is obtained from 7.2.3.26 for the time rate of change of the reduced density matrix

$$\dot{\rho}(t) = -itr_R(\mathscr{L}(t)\bar{W}(t)) - \int_0^t dstr_R\left(\mathscr{L}(t)\mathscr{G}(t,s)(1-\mathscr{P}(s))\mathscr{L}(s)\bar{W}(s)\right). \tag{7.2.3.29}$$

By writing the Liouvilian 7.2.3.19 in the form

$$\mathscr{L}(t) = \frac{1}{\hbar}[\mathscr{H} - \mu(t), \%] + \frac{1}{\hbar}[\mu(t) + H_{ext}(t), \%] \tag{7.2.3.30}$$

where the first term commutes with $\bar{W}(t)$. Using Eq. 7.2.3.9, it is found that

$$tr_R(\mathscr{L}(t)\bar{W}(t)) = -\frac{1}{\hbar}[\rho(t), \mu(t) + H_{ext}(t)]. \tag{7.2.3.31}$$

Furthermore, the identity

$$[A, e^B] = \int_0^1 d\phi e^{\phi B}[A,B]e^{(1-\phi)B} \tag{7.2.3.32}$$

gives by virtue of 7.2.3.8, 7.2.3.11 and 7.2.3.20

$$\begin{aligned}\mathscr{L}(t) = \bar{W}(t) &= -\beta\mathscr{K}(t)\mathscr{L}(t)(\mathscr{H} - \mu(t)) \\ &= \beta\mathscr{K}(t)\mathscr{L}(t)(\mu(t) + H_{ext}(t)).\end{aligned} \tag{7.2.3.33}$$

Now, by making use of Eqs 7.2.3.31 and 7.2.3.33, the evolution of equation 7.2.3.29 may be transformed to

$$\dot{\rho}(t) = -\boldsymbol{V}(t)(\mu(t) + H_{ext}(t)) - \int_0^1 ds\boldsymbol{D}(t,s)(\mu(s) + H_{ext}(s)), \tag{7.2.3.34}$$

where we have introduced the transport operators

$$\boldsymbol{V}(t)u = -\frac{1}{\hbar}[\rho(t), u] \tag{7.2.3.35}$$

and

$$\boldsymbol{D}(t,s)u = \beta tr_R\left(\mathscr{L}(t)\mathscr{G}(t,s)(1-\mathscr{P}(s))\mathscr{K}(s)\mathscr{L}(s)u\right) \tag{7.2.3.36}$$

where $\boldsymbol{V}(t)$ describes the instantaneous transport while $\boldsymbol{D}(t,s)$ describes the retarded transport caused by forces at earlier times. Their time dependence arises only through $\mu(t)$ and $H_{ext}(t)$ Equation 7.2.3.34 is an exact evolution equation (generalized master equation) for the density matrix $\rho(t)$ of the subsystem S, which is nonlinear. This nonlinearity is a pure quantum effect.

At this point, we deal with the problem of finding an approximate equation of motion in cases where memory effects may be disregarded. Such an approximation is conveniently split into two parts. First, we aim at an approximate expression for the thermodynamic force operator $\mu(t)$ in terms of the density matrix $\rho(t)$. This amounts to an approximate description of the static behavior of S. Second, approximate expressions for the transport operators describing the dynamic behavior are sought for. The result of this investigation is the Markovian master equation, which will be showed later on. The thermodynamic force operator $\mu(t)$ introduced in 7.2.3.8 is determined by the requirement 7.2.3.9. We now assume that this relation between $\mu(t)$ and $\rho(t)$ can be replaced by

$$\rho(t) = N(t)e^{-\beta(H-\mu(t)}, \qquad N(t) = tr\left(e^{-\beta(H-\mu(t))}\right) \tag{7.2.3.37}$$

where H has been introduced earlier in Eq. 7.2.3.6. This approximation amounts to the assumption that the steady state of S in the presence of a time-independent perturbation H_{ext} is of the form

$$\rho_{st} \sim e^{-\beta(H+H_{ext})}. \tag{7.2.3.38}$$

While this formula is precise for classical systems, it is valid only approximately in the quantal case. The effective Hamiltonian H characterizing the equilibrium state of S contains frequency shifts due to the interaction with R. When a perturbation H_{ext} is applied to S, the bath state is perturbed by the combined action of H_{ext} and the coupling between S and R. The modified bath state reacts upon S leading to a small change of the effective Hamiltonian. This indirect effect of the perturbation, mediated by the bath, is disregarded in 7.2.3.38. Using the approximate result 7.2.3.37, we obtain instead of 7.2.3.14

$$\delta\rho = \beta\boldsymbol{K}(t)\delta\mu(t) \tag{7.2.3.39}$$

where

$$\begin{aligned}\boldsymbol{K}(t)u &= (N(t)\beta)^{-1}\int\limits_0^\beta d\alpha(e^{-\alpha}(H-\mu(t))ue^{-(\beta-\alpha)(H)-\mu(t)}) \\ &= \int\limits_0^1 dx\rho(t)^x u\rho(t)^{1-x}\end{aligned} \tag{7.2.3.40}$$

is a special type of multiplication with the density matrix $\rho(t)$ which in the classical limit reduces to an ordinary multiplication. Note that $\boldsymbol{K}(t)u$ is self adjoint if u is selfadjoint.

The transport operator $\boldsymbol{V}(t)$ describes the reversible organized motion of S. Since $H - \mu(t)$ commutes with $\rho(t)$, we obtain from 7.2.3.35 and 7.2.3.37

$$-\boldsymbol{V(t)}(\mu(t) + H_{ext}) = -\frac{i}{\hbar}[H + H_{ext}(t), \rho(t)] = -i\boldsymbol{L_0}(t)\rho(t) \tag{7.2.3.41}$$

where $\boldsymbol{L_0}(t)$ is the reversible Liouvillian. Thus the internal reversible dynamics are governed by the effective Hamiltonian H. The transport operator $\boldsymbol{D}(t,s)$ introduced in Eq. 7.2.3.36 reads

$$\boldsymbol{D}(t,s)u = \beta tr_R\left(\mathscr{L}(t)(1 - \mathscr{P}(t))\mathscr{G}(t,s)(1 - \mathscr{P}(s))\mathscr{K}(s)\mathscr{L}(s)u\right) \tag{7.2.3.42}$$

where the term $(1 - \mathscr{P}())$ has been inserted and is permitted because of Eq. 7.2.3.18a. The Hamiltonian $\mathscr{H}(t)$ of $S \otimes R$ can be split into

$$\mathscr{H}(t) = H_S + H_R + \prime H + H_{ext}(t) \tag{7.2.3.43}$$

The interaction $\prime H$ between S and R may be written as

$$\prime H = \sum_l S_l R_l \tag{7.2.3.44}$$

where S_l and R_l are variables of S and R respectively. Then, ot is shown that

$$tr_R\left(\mathscr{L}(t)(1 - \mathscr{P}(t))U\right) = \frac{1}{\hbar}\sum_l [S_l, tr_R(R_l(1 - \mathscr{P}(t))U)] \tag{7.2.3.45}$$

and

$$(1 - \mathscr{P}(s))\mathscr{K}(s)\mathscr{L}(s)u = \frac{1}{\hbar}(1 - \mathscr{P}(s))\mathscr{K}(s)\int_l R_l[S_l, u] \tag{7.2.3.46}$$

where U is an operator of $S \otimes R$ while u is an operator of S. Using the above equations **??** and 7.2.3.46, the transport operator 7.2.3.42 may be transformed into

$$\boldsymbol{D}(t,s)u = \sum_{l,m} \frac{1}{\hbar^2}[S_l, \beta\boldsymbol{D}_{l,m}(t,s)\boldsymbol{k}(s)[S_m, u]] \tag{7.2.3.47}$$

where the diffusion operators have been introduced

$$\boldsymbol{D}_{lm}(t,s) = tr_R\left(R_l(1 - \mathscr{P}(t))\mathscr{G}(t,s)(1 - \mathscr{P}(s))\mathscr{K}(s)\boldsymbol{k}(s)^{-1}R_m\right) \tag{7.2.3.48}$$

So far, all expressions for $\boldsymbol{D}(t,s)$ are exact. We shall assume now, that the motion of the subsystem S is slow compared to the reservoir motion. This means that (in terms of properly scaled variables) the commutator $[S_l, u]$ may be regarded as small in comparison to a commutator of reservoir variables. Since 7.2.3.47 contains two S_l-commutators explicitly, we may evaluate 7.2.3.48 by treating the variables of S as c-numbers. We mention that the diffusion operators will depend on the state of the system S in general. A related phenomenon is met within the theory of classical irreversible systems, where the state-dependence of the diffusion kernels describes multiplicative thermal noise. To keep things as simple as possible, this state-dependence will be disregarded. Finally, we disregard the retardation in the generalized master equation, since memory effects are of the third order in the slowness parameter of S. This way, we obtain after some algebra the Markovian approximation

$$\int 0tds\boldsymbol{D}_{lm}(t,s) = \boldsymbol{k}(s)[S_m, \mu(s) + H_{ext}(s)] = D_{lm}\boldsymbol{K}(t)[S_m, \mu(t) + H_{ext}(t)] \quad (7.2.3.49)$$

where $\boldsymbol{Kt}$ has been defined in 7.2.3.40. The diffusion coefficients D_{lm} are time-integrals over canonical correlations of reservoir variables

$$D_{lm} = \int\limits_0^\infty dt \frac{1}{\beta} \int\limits_0^\beta d\alpha \, \langle \delta R_l(t - i\hbar\alpha)\delta R_m \rangle_R \quad (7.2.3.50)$$

where

$$\delta R_l = R_l - \langle R_l \rangle_R \, . \quad (7.2.3.51)$$

Instead od D_{lm} it is convenient to introduce damping coefficients γ_{lm} by

$$D_{lm} = k_B T \gamma_{lm} \quad (7.2.3.52)$$

because the γ_{lm}, remain finite in the low temperature limit $T \to 0$. By virtue of Eqs 7.2.3.47, 7.2.3.49 and 7.2.3.52 the generalized master equation 7.2.3.34 reduces to the approximate Markovian master equation

$$\dot{\rho}(t) = -\boldsymbol{R}(t)(\mu(t) + H_{ext}(t)) \quad (7.2.3.53)$$

where $\boldsymbol{R}(t)$ is the transport operator in the Markovian limit. It consists of two parts, a commutator

$$\boldsymbol{V}(t) = -\frac{i}{\hbar}[\rho(t), \%] \quad (7.2.3.54)$$

and a sum of double commutators

$$\boldsymbol{D}(t) = \frac{i}{\hbar^2} \sum_{l,m} \gamma_{lm} [S_l, \boldsymbol{K}(t)[S_m, \%]]. \quad (7.2.3.55)$$

Equation 7.2.3.53 has the form of a transport equation. The thermodynamic force operator $\mu(t)$ driving the system to equilibrium is related to the density matrix $\rho(t)$ by 7.2.3.37. The Markovian master equation 7.2.3.53 may also be written in a different form. Using the identity 7.2.3.32 and Eq. 7.2.3.40 one shows that

$$[S_m, \rho(t)] = -\beta \boldsymbol{K}(t)[S_m, H - \mu(t)] \quad (7.2.3.56)$$

from which on can find

$$\boldsymbol{D}(t)\mu(t) = \frac{i}{\hbar^2} \sum_{l,m} \gamma_{lm} [S_l, \boldsymbol{K}(t)[S_m, H] + k_B T [S_m, \rho(t)]]. \quad (7.2.3.57)$$

In the case that no external perturbation is applied, it is obtained from 7.2.3.53 by means of 7.2.3.41 and 7.2.3.57 the following

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho(t)] - \frac{i}{\hbar} \sum_{l,m} \gamma_{lm} [S_l, \boldsymbol{K}(t)\dot{S}_m] - \frac{k_B T}{\hbar^2} \sum_{l,m} \gamma_{lm} [S_l, [S_m, \rho(t)]] \quad (7.2.3.58)$$

where

$$\dot{S}_m = \frac{i}{\hbar}[H, S_m]. \tag{7.2.3.59}$$

Since in the second term on the right hand side of Eq. 7.2.3.58 the dependence on $\rho(t)$ arises through the multiplication operator $\boldsymbol{K}(t)$, Eq. 7.2.3.58) is not a linear equation.

The main results Eq. 7.2.3.53 is exactly of the form of Eq. 7.2.2.23 for the special case of a heat bath as classical environment, that is, with constant coefficients $[H_e, S_e]_x^Q$ and $[H_e, H_e]]_x^Q = Te[H_e, S_e]]_x^Q$ and without the accompanying feedback equation 7.2.2.22 for the evolution of the classical environment. It is quite remarkable that the detailed projection operator derivation from statistical mechanics provides exactly the same non-linear quantum master equation as the application of Diracs method of classical analogy to the geometric formulation of nonequilibrium thermodynamics.

7.2.4 Applied Thermodynamic Quantum Master Equation

The quantum master equation describing the evolution of the density matrix (or statistical operator) ρ of a quantum subsystem in contact with a classical environment in state x is

$$\frac{\partial\rho}{\partial t} = \frac{i}{\hbar}[\rho, H_s] - \frac{1}{k_B}\sum_k [H_e, S_e]_x^{\boldsymbol{Q}_k}[\boldsymbol{Q}_k, [\boldsymbol{Q}_k, H_s]_\rho] - \sum_k [H_e, H_e]_x^{\boldsymbol{Q}_k}[\boldsymbol{Q}_k, [\boldsymbol{Q}_k, \rho]] \tag{7.2.4.1}$$

The first term describes the reversible contribution to the evolution generated by the Hamiltonian H of the quantum subsystem via the commutator. The remaining terms are of irreversible nature and arise due to the coupling of the quantum subsystem to its environment and lead to non-unitary evolution of indicating that we go beyond the simple Schrödinger-type of evolution of closed quantum systems. If the latter terms would be absent (equal to zero), the resulting master equation would reduce to the well-known Lindblad form describing the most general dynamics of a quantum subsystem exposed to an environment under linearity and Markovian assumptions. The irreversible terms are expressed through double commutators involving the self-adjoint coupling operator Q so that the normalization condition, $Tr(\rho) = 1$, is automatically preserved in time. As a consequence of the occurrence of commutators with the coupling operator Q, the evolution of the average $\langle Q\rangle_\rho$ performed with the time-dependent density matrix ρ is not explicitly affected by the dissipative terms.

As we mentioned, the type of coupling to the environment is characterized by the self-adjoint operators Q_k, whereas the corresponding coupling strength is given by the dissipative brackets $[\cdot,\cdot]_x^{Q_k}$, defined as a binary operation on the space of observables for the classical environment . If the equilibrium or non-equilibrium states of the environment are characterized by state variables x, classical observables are functions or functionals of x, and their evaluation at a particular point of the state space is indicated by the subscript x. The classical observables H_e and S_e in Eq. 7.2.4.1 are the energy and the entropy of the environment, respectively. Dissipative brackets are commonly used to characterize the entropy production rate in nonequilibrium thermodynamics [11], [28]. They are characterized by the following properties:
$[A_e, B_e]$ is bilinear in A_e and B_e, is symmetric

$$[A_e, B_e] = [B_e, A_e], \tag{7.2.4.2}$$

as well as non-negative

$$[A_e, B_e] \geq 0, \tag{7.2.4.3}$$

and satisfies the Leibniz or product rule

$$[A_e B_e, C_e] = A_e[B_e, C_e] + B_e[A_e, C_e], \tag{7.2.4.4}$$

for arbitrary environmental variables A_e, B_e, and C_e.

The non-linear part is embedded in the commutator $[Q_k, H]_\rho$. The subscript ρ below an operator A indicates a compromise of placing the density matrix on the right and on the left of this operator,

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda. \tag{7.2.4.5}$$

In standard approaches [2], [6] the Liouvillian of quantum master equations contains terms in which the density matrix ρ is placed on the right site, the left site, or alternatively in between two coupling operators, but not on both sites of an operator simultaneously. The structural element 7.2.4.5 includes this possibility. The resulting non-linear term $[Q_k, [Q_k, H]_\rho]$ improves the relaxation behaviour of solutions and guarantees for the proper long-time behaviour in case the classical environment is a heat bath [8]. The non-linear terms in the quantum master equation, Eq. 7.2.4.1, appear in the form A_ρ. To understand their structure, we make use of the spectral decomposition of the density matrix,

$$\rho = \sum_n p_n \left|\pi_n\right\rangle \left\langle\pi_n\right|, \tag{7.2.4.6}$$

where, p_n and $|\pi_n\rangle$ are the eigenvalues and orthonormal eigenvectors of the statistical operator ρ, respectively. By performing the integration in Eq. 7.2.4.5, one obtains the following identity [8], [12]

$$A_\rho = \sum_{m,n} \frac{p_m - p_n}{\ln p_m - \ln p_n} A^\pi_{mn} \left|\pi_m\right\rangle \left\langle\pi_n\right|, \tag{7.2.4.7}$$

where $A^\pi_{mn} = \langle \pi_m \,|\, A \,|\, \pi_n \rangle$ are the matrix elements of A in the eigenbasis of the density matrix. The factor in front of A^π_{kl} in Eq. 7.2.4.7 we have the inequalities

$$\sqrt{p_m p_n} \leq \frac{p_m - p_n}{\ln p_m - \ln p_n} \leq \frac{p_m + p_n}{2}, \tag{7.2.4.8}$$

so that no problems occur for $p_m = p_n$. If p_m or p_n or both of them go to zero, also this factor goes to zero. Moreover, like the bounds, the factor in the middle of Eq. 7.2.4.8 changes monotonically with p_m, $p_n \in [0,1]$. The operator A_ρ can be decomposed into its linear and non-linear contributions by means of

$$A_\rho = \frac{1}{2}\left(A\rho + \rho A + \int_0^1 [\rho^\lambda, [\rho^{1-\lambda}, A]] d\lambda \right). \tag{7.2.4.9}$$

If we neglect the last term in Eq. 7.2.4.9, then the master equation 7.2.4.1 becomes linear. This linearization is not recommended [8] as it spoils the overall structure of the thermodynamic approach. As a consequence of this linearization, the proper equilibrium solution is not guaranteed in case of a heat bath environment.

In a heat bath environment the quantum subsystem cannot have any influence on the state x of the environment. The complete thermodynamic information of the classical environment is encoded in the thermodynamic potentials. For convenience, we do this description in terms of the entropy $S_e(H_e)$ which we use directly as the state variable x. By means of the relation

$$\frac{1}{T_e} = \frac{\partial S_e}{\partial t} \tag{7.2.4.10}$$

we can assign a temperature T_e to the heat bath. The most general form of the dissipative bracket for a heat bath is given by

$$[A_e, B_e]_{S_e}^{Q_k} = \frac{dA_e}{dH_e} M_k(T_e) \frac{dB_e}{dH_e}, \tag{7.2.4.11}$$

where H_e can be obtained by Legendre transformation from S_e. The functions $M_k(T_e)$ and must be symmetric, positive semi-definite and satisfy the Leibniz rule. By combining the previous equations, the heat bath obeys

$$T_e[H_e, S_e]_x^{\boldsymbol{Q}_k} = [H_e, H_e]_x^{\boldsymbol{Q}_k} \tag{7.2.4.12}$$

This condition allows to write down all classical brackets appearing in the thermodynamic quantum master equation 7.2.4.1 once the friction structures M^j are known, so that these carry the complete knowledge about the coupling strength between the quantum subsystem and the environment:

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar}[\rho, H_s] - \sum_k \frac{1}{k_B T_{e,k}} M_k(T_{e,k})[\boldsymbol{Q}_k, [\boldsymbol{Q}_k, H_s]_\rho] - \sum_k M_k(T_{e,k})[\boldsymbol{Q}_k, [\boldsymbol{Q}_k, \rho]]. \tag{7.2.4.13}$$

It can be shown that the stationary solution of the quantum master equation, Eq. 7.2.4.13, is the Boltzmann distribution $\rho_{eq} \propto exp(-\frac{H}{k_B T_e})$ The guaranteed existence of this solution is a direct consequence of the special form of the non-linear part $[Q_k, H]_\rho$ in the quantum master equation [8].

The general thermodynamic approach also provides an equation for the entropy production [8]. The average $\bar{S}$ of the total entropy of the quantum subsystem and its classical environment evolves according the equation

$$\frac{d\bar{S}}{dt} = -k_B Tr\left(ln\rho \frac{d\rho}{dt}\right) + \frac{dS_{e,x}}{dt}. \tag{7.2.4.14}$$

For two pure heat baths at temperature T_l and T_r, by construction of the dissipative bracket the entropy production can be expressed in terms of the canonical correlation

$$\frac{d\bar{S}}{dt} = \sum_{k=l,r} \frac{M(T_k)}{k_B {T_k}^2} \langle i[Q_k, F_k]; i[Q_k, F_k]\rangle_\rho \tag{7.2.4.15}$$

where

$$F_k = H_s + k_B T_k ln(\rho), \tag{7.2.4.16}$$

is the Helmholtz free energy operator,

$$\begin{aligned} \langle i[Q_k, F_k]; i[Q_k, F_k]\rangle_\rho &= -\langle [Q_k, F_k]; [Q_k, F_k]\rangle_\rho \\ &= -Tr\left([Q_k, F_k]_\rho [Q_k, F_k]\right) \end{aligned} \tag{7.2.4.17}$$

The dissipative brackets are assumed to be given by the friction functions

$$M_k(T_{e,k}) = \gamma_k T_{e,k} \tag{7.2.4.18}$$

Then, the non-linear thermodynamic quantum master equation 7.2.4.13 reads

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H_S, \rho] - \sum_{k=l,r} \gamma_k [\boldsymbol{Q}_k, [\boldsymbol{Q}_k, H_S]_\rho] - \sum_{k=l,r} \gamma_k T_{e,k} [\boldsymbol{Q}_k, [\boldsymbol{Q}_k, \rho]] \tag{7.2.4.19}$$

7.2.5 Three-Level System (Qutrit)

In the case of the three-level system, the form of the quantum master equation is of Eq. 7.2.4.19, where the coupling operators Q_k $(k = l, r)$ being 3×3 matrices, to be defined later.

7.2.6 Harmonic Oscillator (10 states)

Similarly to the previous case, when the quantum subsystem is a harmonic oscillator the form of the quantum master equation is of Eq. 7.2.4.19, where the coupling operators Q_k $(k = l, r)$ being 10×10 matrices, to be defined later.

7.3 Steady-State Effective Temperatures

Having the steady-state solutions in our hands for the density matrix, we can now compute the Effective Temperatures of the systems from the following relation

$$\begin{aligned}
&\frac{\rho_{ii,ss}}{\rho_{jj,ss}} = e^{-\beta_{ij}(E_i - E_j)} \Leftrightarrow \\
&\beta_{ij} = -\frac{1}{E_i - E_j} ln\left(\frac{\rho_{ii,ss}}{\rho_{jj,ss}}\right) \Leftrightarrow \\
&T_{ij} = -\frac{E_i - E_j}{ln\left(\frac{\rho_{ii,ss}}{\rho_{jj,ss}}\right)},
\end{aligned} \tag{7.3.1}$$

which are as many as are the states of the system under study.

7.4 Heat Flux

Regardless what is the investigating quantum system, we have to respect some general laws. In that sense, we have to somehow identify that the derived results are the expected ones and lie on a reasonable basis. Someone might find enough ways to clarify this issue. Although, consistency check which in our case illustrate this exact thing is that the total heat flux of the open system is equal to zero. Consequently, this means that the corresponding heat flux which enters the quantum system due to the heat bath with the highest temperature values is equal to the one that exits the system towards the other heat bath.

In order to do the above consistency check, the following relations must hold, depending on case that we study.

- **Lindblad Master Equation**

  We define as the amount of heat flux reffering to each heat bath k as

  $$J_k^{LME}(t) = Tr\left(H_S \mathcal{K}_k\left(\rho(t)\right)\right) \tag{7.4.1}$$

  Hence, the total heat flux of the system is the sum of the above

  $$J^{LME}(t) = \sum_k J_k^{LME}(t) = \sum_{k=l,r)} Tr\left(H_S \mathcal{K}_k\left(\rho(t)\right)\right) \tag{7.4.2}$$

- **Non-Linear Thermodynamic Quantum Master Equation**

  Likewise the previous case, the heat flux of corresponding to each heat bath k is given by

  $$J_k^{TQME}(t) = Tr\left(H_S\left(\gamma_k[Q_k,[Q_k,H_S]_\rho] + \gamma_k T_{e,k}[Q_k,[Q_k,\rho]]\right)\right) \tag{7.4.3}$$

  Consequently, the total heat flux of the system is given by

  $$J^{TQME}(t) = \sum_k J_k^{TQME}(t). \tag{7.4.4}$$

In both cases, the consistency check that we perform is that the following relation must hold in steady-state

$$J^{LME}(t \to \infty) = 0 \tag{7.4.5}$$

and

$$J^{TQME}(t \to \infty) = 0. \tag{7.4.6}$$

which means that when the system reaches equilibrium, the total heat flux is equal to zero and the individual ones are equal of opposite sign.

Chapter 8

Numerical Methods

In this section, we are going to present the numerical methods that were implemented for the solution of both master equations; the Lindblad-type of and the thermodynamic quantum master equation. Each of them were applied to the case of the three-level and harmonic oscillator quantum system, coupled each time to two heat baths of different temperatures.

8.1 Adams-Bashforth method

Linear multi-step methods are used for the numerical solution of ordinary differential equations. Conceptually, a numerical method starts from an initial point and then takes a short step forward in time to find the next solution point. The process continues with subsequent steps to map out the solution. Single-step methods (such as Euler's method of the form $y_{n+1} = y_n + hf(t_n, y_n)$) refer to only one previous point and its derivative to determine the current value. Methods such as Runge-Kutta take some intermediate steps (for example, a half-step) to obtain a higher order method, but then discard all previous information before taking a second step. Multi-step methods attempt to gain efficiency by keeping and using the information from previous steps rather than discarding it. Consequently, multi-step methods refer to several previous points and derivative values. In the case of linear multi-step methods, a linear combination of the previous points and derivative values is used. Numerical methods for ordinary differential equations approximate solutions to initial value problems of the form

$$y' = f(t, y), \;\; y(t_0) = y_[0]. \tag{8.1.1}$$

The result is approximations for the value of $y(t)$ at discrete times t_i:

$$y_i \approx y(t_i) \text{ where } t_i = t + 0 + ih, \tag{8.1.2}$$

where h is the time step. Multi-step methods use information from the previous s steps to calculate the next value. In particular, a linear multi-step method uses a linear combination of y_i and $f(t_i, y_i)$ to calculate the value of y for the desired current step. Thus, a linear multi-step method is a method of the form

$$\begin{aligned} &y_{n+s} + a_{s-1}y_{n+s-1} + a_{s-2}y_{n+s-2} + \cdots + a_0 y_n \\ &\quad = h\big(b_s f(t_{n+s}, y_{n+s}) + b_{s-1} f(t_{n+s-1}, y_{n+s-1}) + \cdots + b_0 f(t_n, y_n)\big), \end{aligned} \tag{8.1.3}$$

The coefficients $a_0, \dots, a_{s-1}$ and $b_0, \dots, b_s$ determine the method. The designer of the method chooses the coefficients, balancing the need to get a good approximation to the true solution against the desire to get a method that is easy to apply. Often, many coefficients are zero to simplify the method. One can distinguish between explicit and implicit methods. If $b_s = 0$, then the method is called "explicit", since the formula can directly compute y_{n+s} . If $b_s \neq 0$ then the method is called "implicit", since the value of y_{n+s} depends on the value of $f(t_{n+s}, y_{n+s})$, and the equation must be solved for y_{n+s}. Iterative methods such as Newton's method are often used to solve the implicit formula. Sometimes an explicit multi-step method is used to "predict" the value of y_{n+s}. That value is then used in an implicit formula to "correct" the value. The result is a predictorcorrector method. Three families of linear multi-step methods are commonly used: Adams-Bashforth methods, Adams-Moulton methods, and the backward differentiation formulas (BDFs). The Adams-Bashforth-methods are explicit methods. The coefficients are $a_{s-1} = -1$ and $a_{s-2} = \cdots = a_0 = 0$, while the b_j are chosen such that the methods has order s (this determines the methods uniquely). The Adams-Bashforth methods with $s = 1, 2, 3, 4, 5$ are [30], [31] :

$$\begin{aligned}
y_{n+1} &= y_n + hf(t_n, y_n), \qquad \text{(This is the Euler method)} \\
y_{n+2} &= y_{n+1} + h\left(\frac{3}{2}f(t_{n+1}, y_{n+1}) - \frac{1}{2}f(t_n, y_n)\right), \\
y_{n+3} &= y_{n+2} + h\left(\frac{23}{12}f(t_{n+2}, y_{n+2}) - \frac{4}{3}f(t_{n+1}, y_{n+1}) + \frac{5}{12}f(t_n, y_n)\right), \\
y_{n+4} &= y_{n+3} + h\left(\frac{55}{24}f(t_{n+3}, y_{n+3}) - \frac{59}{24}f(t_{n+2}, y_{n+2})\right. \\
&\qquad\qquad \left. + \frac{37}{24}f(t_{n+1}, y_{n+1}) - \frac{3}{8}f(t_n, y_n)\right), \\
y_{n+5} &= y_{n+4} + h\left(\frac{1901}{720}f(t_{n+4}, y_{n+4}) - \frac{1387}{360}f(t_{n+3}, y_{n+3})\frac{109}{30}f(t_{n+2}, y_{n+2})\right. \\
&\qquad\qquad \left. - \frac{637}{360}f(t_{n+1}, y_{n+1}) + \frac{251}{720}f(t_n, y_n)\right).
\end{aligned} \tag{8.1.4}$$

The coefficients b_j can be determined as follows. Use polynomial interpolation to find the polynomial p of degree $s - 1$ such that

$$p(t_{n+i}) = f(t_{n+i}, y_{n+i}), \qquad \text{for } i = 0, \dots, s-1. \tag{8.1.5}$$

The Lagrange formula for polynomial interpolation yields

$$p(t) = \sum_{j=0}^{s-1} \frac{(-1)^{s-j-1} f(t_{n+j}, y_{n+j})}{j!(s-j-1)!h^{s-1}} \prod_{\substack{i=0 \\ i \neq j}}^{s-1} (t - t_{n+i}). \tag{8.1.6}$$

The polynomial p is locally a good approximation of the right-hand side of the differential equation $y' = f(t, y)$ that is to be solved, so consider the equation $y' = p(t)$ instead. This equation can be solved exactly; the solution is simply the integral of p. This suggests taking

$$y_{n+s} = y_{n+s-1} + \int_{t_{n+s-1}}^{t_{n+s}} p(t)\,dt. \tag{8.1.7}$$

The Adams-Bashforth method arises when the formula for p is substituted. The coefficients b_j turn out to be given by

$$b_{s-j-1} = \frac{(-1)^j}{j!(s-j-1)!} \int_0^1 \prod_{\substack{i=0 \\ i\neq j}}^{s-1} (u+i)\, du, \qquad \text{for } j = 0, \ldots, s-1. \tag{8.1.8}$$

Replacing $f(t, y)$ by its interpolant p incurs an error of order hs, and it follows that the s-step Adams-Bashforth method has indeed order s [32] The Adams-Bashforth methods were designed by John Couch Adams to solve a differential equation modelling capillary action due to Francis Bashforth. Bashforth in 1883 published his theory and Adams' numerical method [33].

A major disadvantage of multistep formulas is that they are not self-starting. Thus, in the Adams-Bashforth method with $s = 4$ in Eq. 8.1.4, we must have four successive values of $f(x, y)$ at equally spaced points before this formula can be used. These starting values must be obtained by some independent method. We might, for example, use single-step Euler's method or one of the Runge-Kutta methods to obtain these starting values. We must also be assured that these starting values are as accurate as necessary for the overall required accuracy. A second disadvantage of the Adams-Bashforth method is that, although the local discretization error is $\mathcal{O}(h^5)$, the coefficient in the error term is somewhat larger than for formulas of the Runge-Kutta type of the same order. Runge-Kutta methods are generally, although not always, more accurate for this reason. On the other hand, the multistep formulas require only one derivative evaluation per step, compared with four evaluations per step with Runge-Kutta methods, and are therefore considerably faster and require less computational work [34].

In this work, the Adams-Bashforth method with $s = 4$ in Eq. 8.1.4 (4th order) is used, with the help of single-step Euler's scheme in order to obtain the four starting values. The main reason for choosing this integration scheme to solve the two master equations is because it requires less computational work which is very important, especially in the case the quantum thermodynamic master equation, Eq. 7.2.4.1. The step that were chosen was $h = 10^{-2}$

8.2 Newton-Raphson Method

In numerical analysis, Newton's method (also known as the Newton-Raphson method), named after Isaac Newton and Joseph Raphson, is a method for finding successively better approximations to the roots (or zeroes) of a real-valued function.

$$x : f(x) = 0. \tag{8.2.1}$$

The Newton-Raphson method in one variable is implemented as follows: Given a function f defined over the real x, and its derivative f', we begin with a first guess x_0 for a root of the function f. Provided the function satisfies all the assumptions made in the derivation of the formula, a better approximation x_1 is

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}. \tag{8.2.2}$$

The process is repeated as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \tag{8.2.3}$$

until a sufficiently accurate value is reached.

In our implementation, we have a set of partial differential equations, corresponding to the density matrix elements. Under steady-state condition, these equations become algebraic and we write them in the residual form. We express each such equation, referring to a density matrix element, to the real and imaginary component. So we have a set of $2 \times d$ equations, where d is the dimension of the density matrix in each case. So, we have the following

$$F(\boldsymbol{x}^i) = 0, \tag{8.2.4}$$

where $\mathbf{x}$ is the vector of unknown of dimension $2 \times d$. The first step is to calculate the function values at a guessed, initial value, x^i. Later on, we compute the Jacobian matrix, J, at the current guess for the solution. Afterwards, we solve the linear system

$$Jd\mathbf{x} = -F(\boldsymbol{x}^i) \tag{8.2.5}$$

using LU decomposition, for the values of $d\mathbf{x}$ and then we update the guessed value

$$\boldsymbol{x}^{i+1} = \boldsymbol{x} + d\boldsymbol{x}. \tag{8.2.6}$$

This procedure should be repeated, using the updated value of $\mathbf{x}^{\mathbf{i}}$ as the guess, until the values of the residual vector, $F(\boldsymbol{x})$ are sufficiently close to zero.

CHAPTER 9

NON-DIMENSIONALIZATION - INPUTS

9.1 Non-Dimensionalization

The dimensionless form of the thermodynamic quantum master equation 7.2.4.19 is the following:

$$\frac{\partial \tilde{\rho}}{\partial \tilde{t}} = -i[\tilde{H}_S, \tilde{\rho}] - \gamma_k [Q_k, [Q_k, \tilde{H}_S]_\rho] - \gamma_k \tilde{T_e, k}[Q_k, [Q_k, \tilde{\rho}]] \tag{9.1.1}$$

where

- $\omega_0 \equiv \omega$
- $\tilde{t} = t\omega_0$
- $\tilde{H}_S = \frac{H_S}{\hbar\omega_0}$
- $T_0 = \frac{\hbar\omega_0}{k_B}$
- $\tilde{T}_{e,k} = \frac{T_{e,k}}{T_0} = \frac{T}{T_0}$

Specification of the characteristic frequency ω_0 defines all dimensionless variables.

In this work, the above dimensionless form is applied to the systems of interest, in order to extract our results.

9.2 Inputs

As inputs to the solution of these master equations we have used the following: The chosen Hamiltonian, H_S, of the corresponding system under investigation, is

- Three-Level System (Qutrit)

$$H_S = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0.7 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{9.2.1}$$

  The coupling operators corresponding to the left (l) and the right (r) heat bath are the following:

$$Q_l = \begin{pmatrix} 0 & i & i \\ -i & 0 & i \\ -i & -i & 0 \end{pmatrix}, \tag{9.2.2a}$$

$$Q_r = \begin{pmatrix} 0 & -i & -i \\ i & 0 & -i \\ i & i & 0 \end{pmatrix} \tag{9.2.2b}$$

  where we have chosen $Q_k = {Q_k}^\dagger$ for $k = l, r$.

- Harmonic Oscillator (10 states)

$$H_S = \begin{pmatrix} 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.5 \end{pmatrix} \tag{9.2.3}$$

  The coupling operators corresponding to the left (l) and the right (r) heat bath are now the 10×10 matrices:

$$\boldsymbol{Q}_l = \begin{pmatrix} 0 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -i & 0 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -i & 0 & i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i & 0 & i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -i & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -i & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i & 0 & i \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i & 0 \end{pmatrix} \tag{9.2.4a}$$

$$\boldsymbol{Q}_r = \begin{pmatrix} 0 & -i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ i & 0 & -i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & i & 0 & -i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & -i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i & 0 & -i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & i & 0 & -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & i & 0 & -i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & i & 0 & -i \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & i & 0 \end{pmatrix} \tag{9.2.4b}$$

where $\boldsymbol{Q}_k = \boldsymbol{Q}_k{}^{\dagger}$ for $k = l, r$.

At this point, it is important to note that the ij elements of the coupling operators Q_k (Q_k^{ij}) that were used in order to define the Lindblad operators in 7.1.1.2 and 7.1.2.3 in the case of the Lindblad master equation 7.1.2, are condensed in a matrix Q_k where is the one that we defined above and are used in the thermodynamic quantum master equation.

The temperature of the two heat baths were selected to be different to each other and equal to $T_{e,l} = 0.4$, for the left, and $T_{e,r} = 0.8$ for the right one. As for the friction coefficient, $\gamma_l = \gamma_r = 0.01$ assuming weak coupling with the environment . Also, we assume $\hbar = \omega = k_B = 1$. The values of the coupling operators in each occasion have been given earlier, in Eq. 9.2.2 and Eq. 9.2.4.

The initial condition used in both systems is that all the population is initially in the ground state, i.e. at $t = 0$ the $(1, 1)$ element of the density matrix is equal while all the other element are equal to zero.

An important note is to check the properties of the density matrix, ρ, and if those properties are fulfilled throughout our calculations. First of all, the diagonal elements have to be real and greater than zero, while the sum of these terms must be equal to one, as they express probability values. Also, the eigenvalues of this matrix each time must be real and positive.

CHAPTER 10

RESULTS

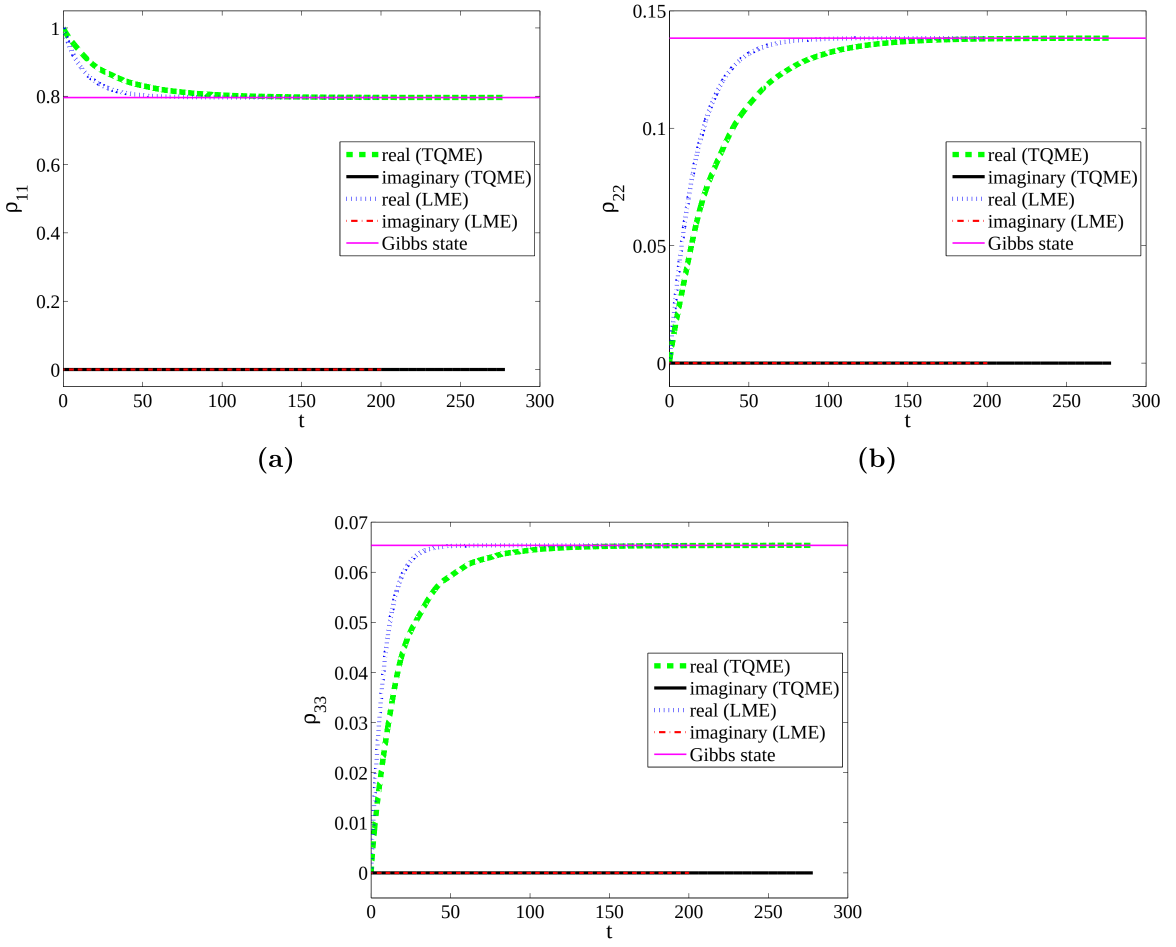
10.1 Quantum Susbsystem coupled to One Heat Bath

In this section, results are presented that have been obtained through the time integration and the direct calculation of the steady-state values using the Lindblad Master Equation (LME), Eq. 7.1.2, and the Thermodynamic Quantum Master Equation (TQME), Eq. 7.2.4.1. These results refer to the two cases that we study; the three-level and the harmonic oscillator as quantum subsystems coupled to one heat bath. The inputs where the same mentioned for the left heat bath only in section 9.2, with $T_e = 0.4$ and $\gamma = 0.01$.

10.1.1 Time Integration

The integration scheme used in this work is the Adams-Bashforth 4th order ($s = 4$) in Eq. 8.1.4) with the help of single-step Euler's scheme in order to obtain the four starting values. The integration time step that we set was $h = 10^{-2}$.

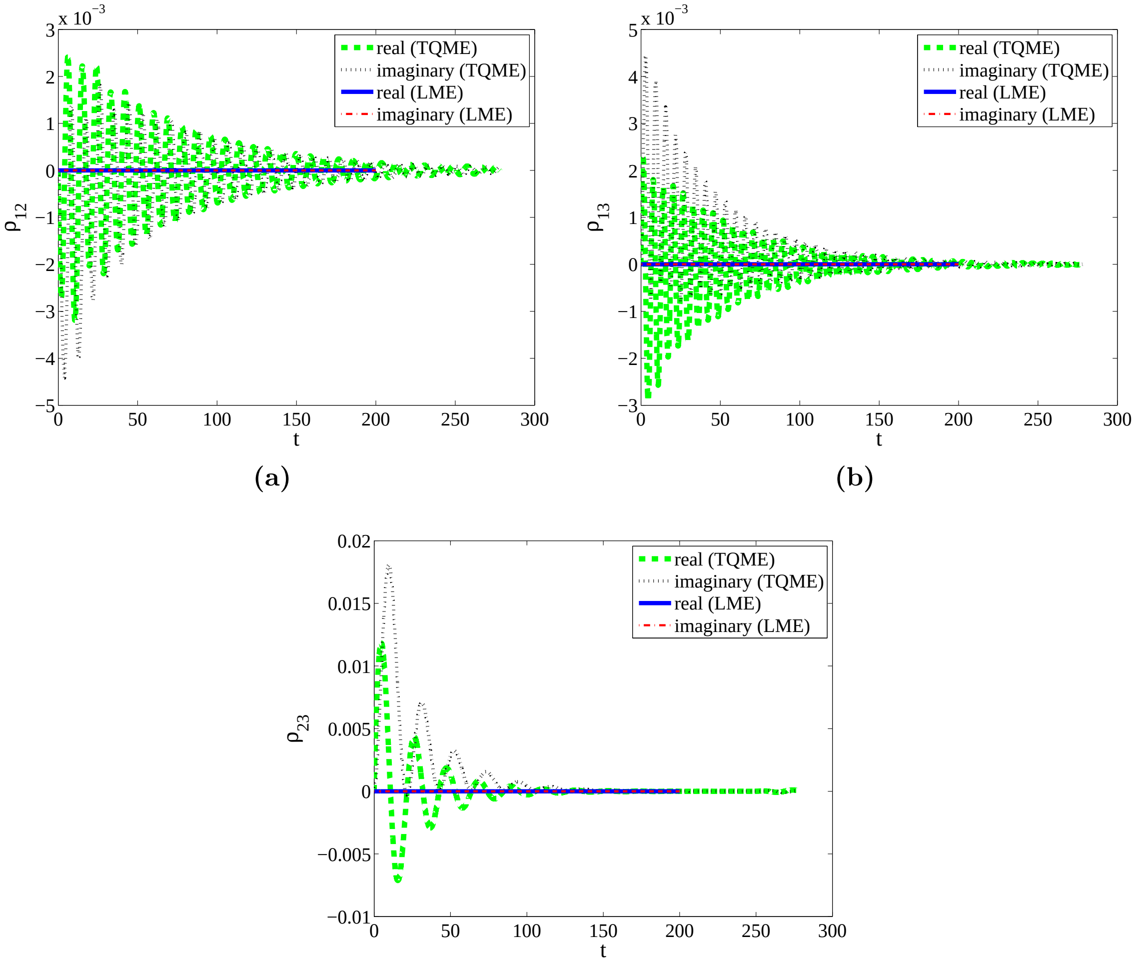
Three-Level System (Qutrit)



(a) **(b)**

(c)

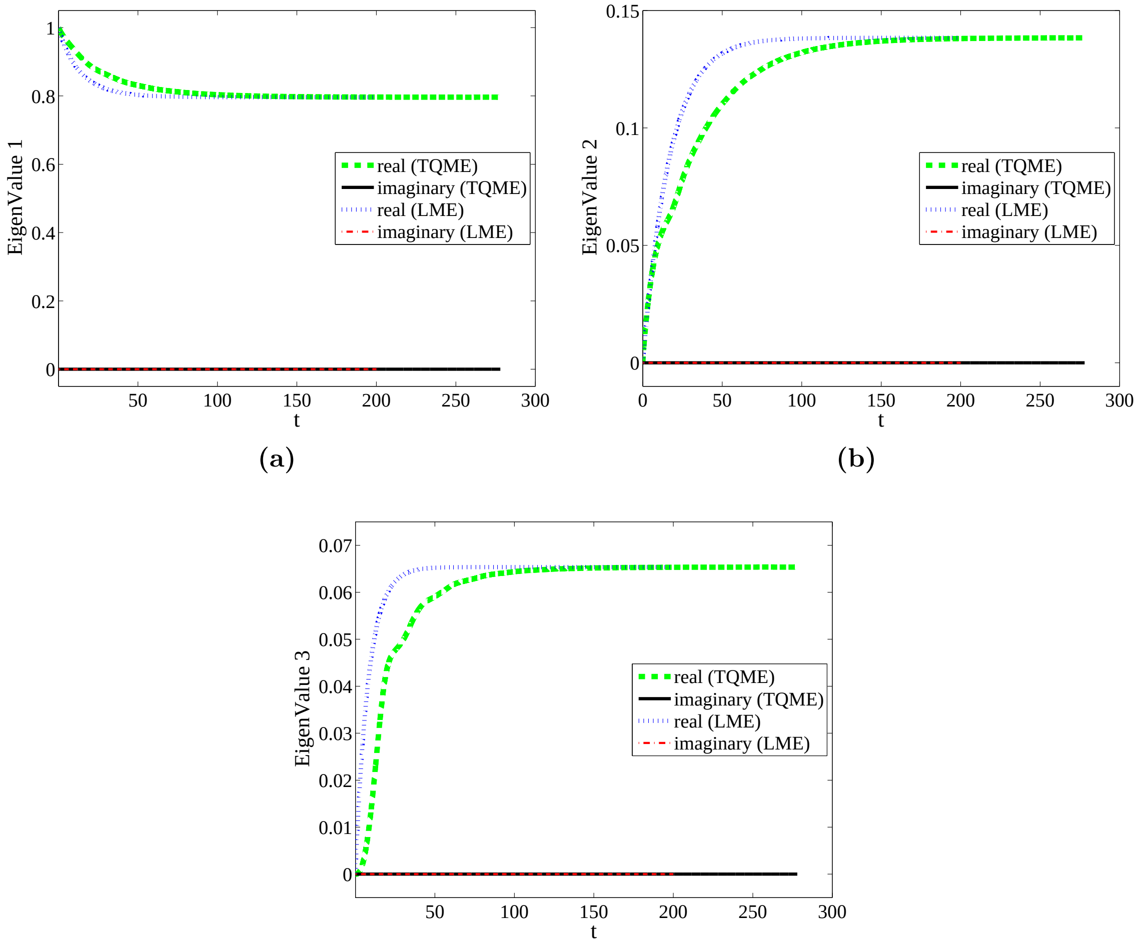
Figure 10.1.1.1: Time evolution of the real and imaginary part of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, using the Lindblad Master Equation (LME) (real (green), imaginary (black)) and the Thermodynamic Quantum Master Equation (TQME) (real (blue), imaginary (red)) for the case of the Three-Level system (Qutrit), with $T_e = 0.4$ and $\gamma = 0.01$.



(a) **(b)**

(c)

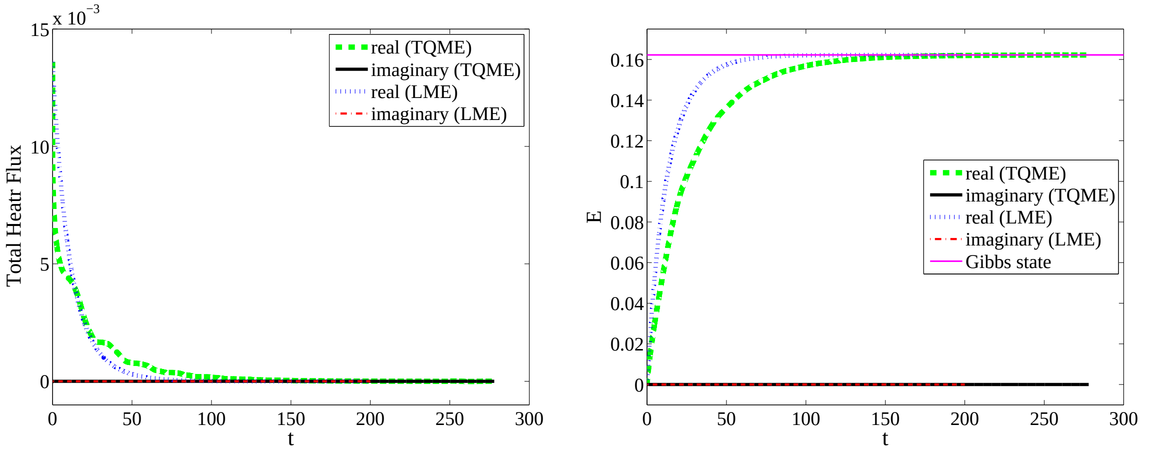
Figure 10.1.1.2: Same as 10.1.1.1 but for the non-diagonal density matrix elements, ρ_{12}, ρ_{13}, ρ_{23}.



(a) **(b)**

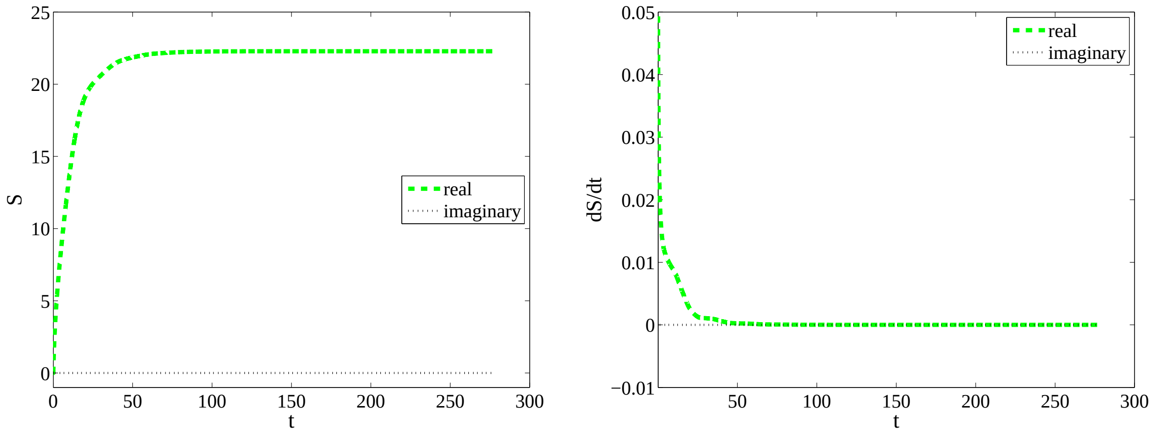
(c)

Figure 10.1.1.3: Same as 10.1.1.1 but for the eigenvalues of the density matrix.



(a) **(b)**

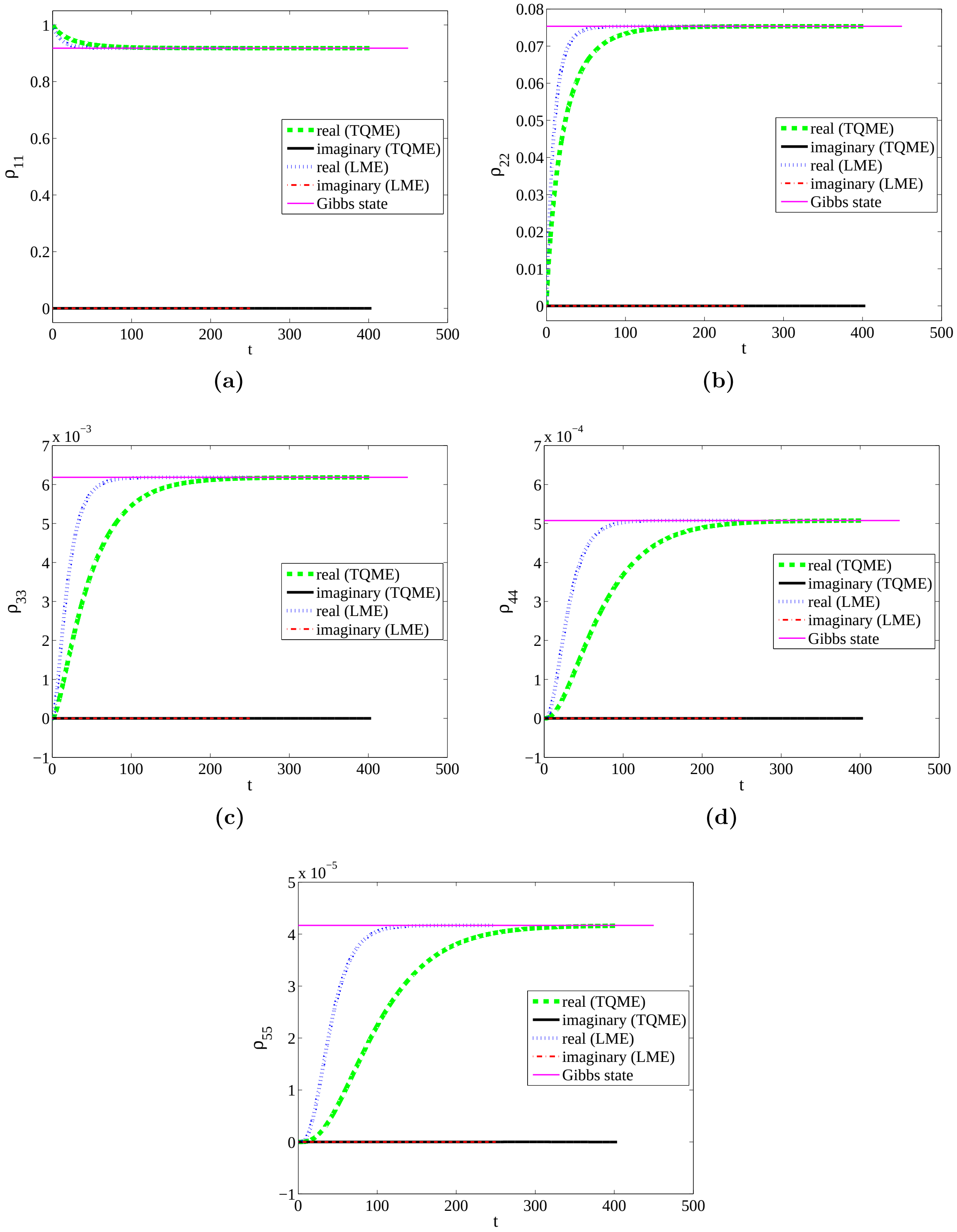
Figure 10.1.1.4: Same as 10.1.1.1 but for the heat flux of the heat bath and the energy E of the system.



(a) **(b)**

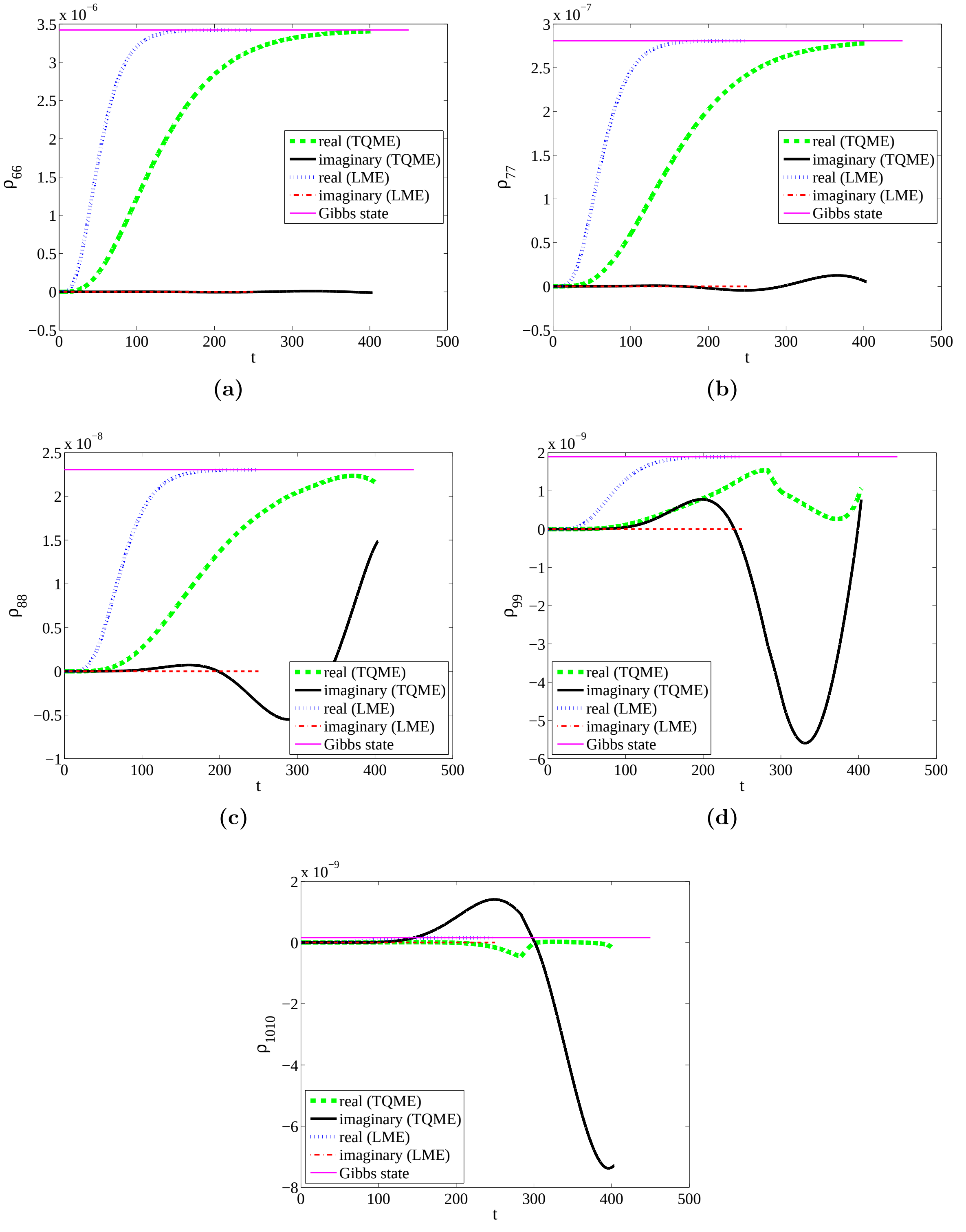
Figure 10.1.1.5: Time evolution of the real and imaginary part of the entropy S of the system and $\frac{dS}{dt}$, using the Thermodynamic Quantum Master Equation (TQME) (real (green), imaginary (black)) for the case of the Three-Level system (Qutrit), with $T_e = 0.4$ and $\gamma = 0.01$.

Harmonic Oscillator (10 states)



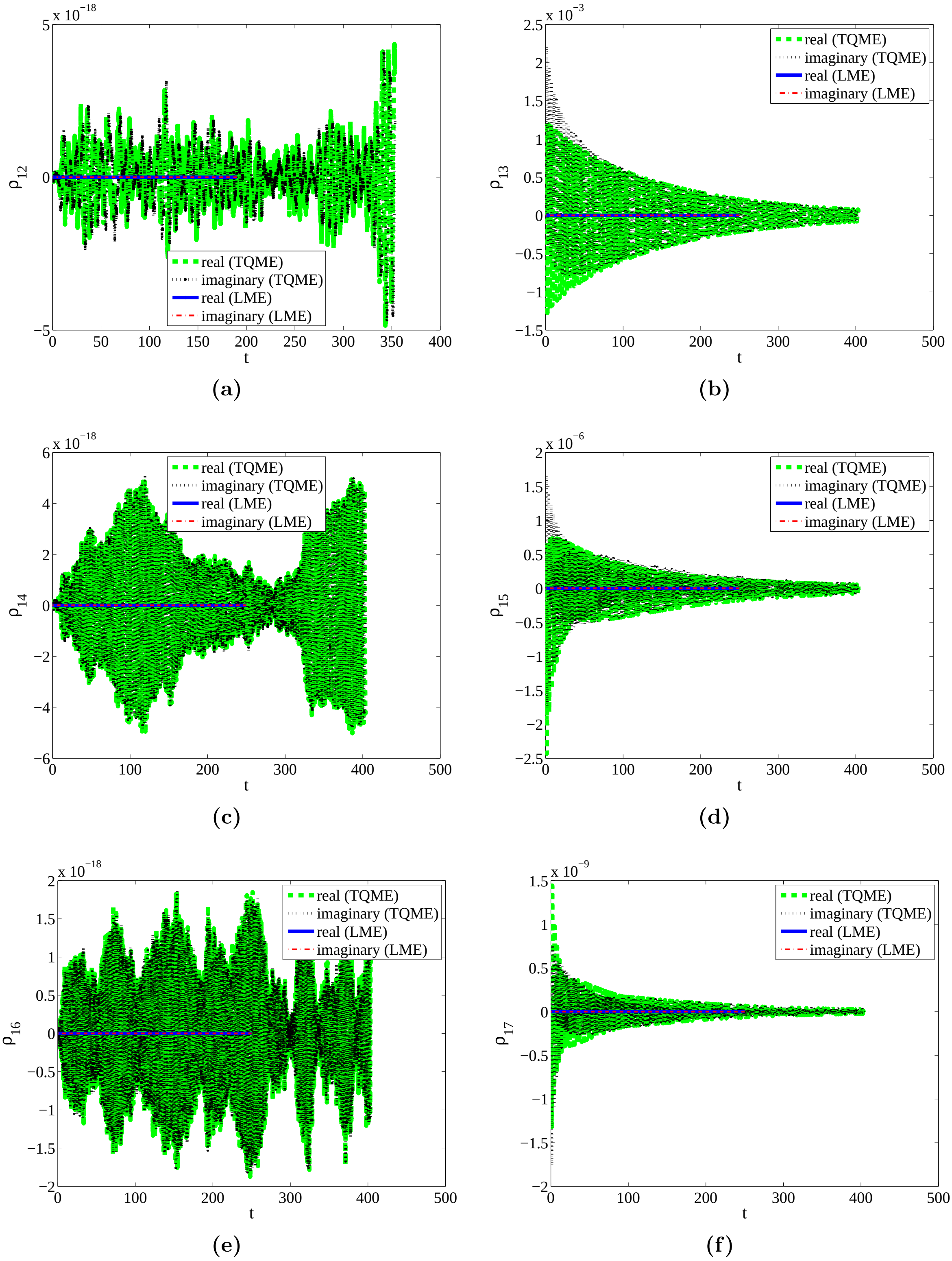
(a) (b) (c) (d) (e)

Figure 10.1.1.6: Time evolution of the real and imaginary part of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, using the Lindblad Master Equation (LME) (real (green), imaginary (black)) and the Thermodynamic Quantum Master Equation (TQME) (real (blue), imaginary (red)) for the case of the Harmonic Oscillator (10 states), with $T_e = 0.4$ and $\gamma = 0.01$.



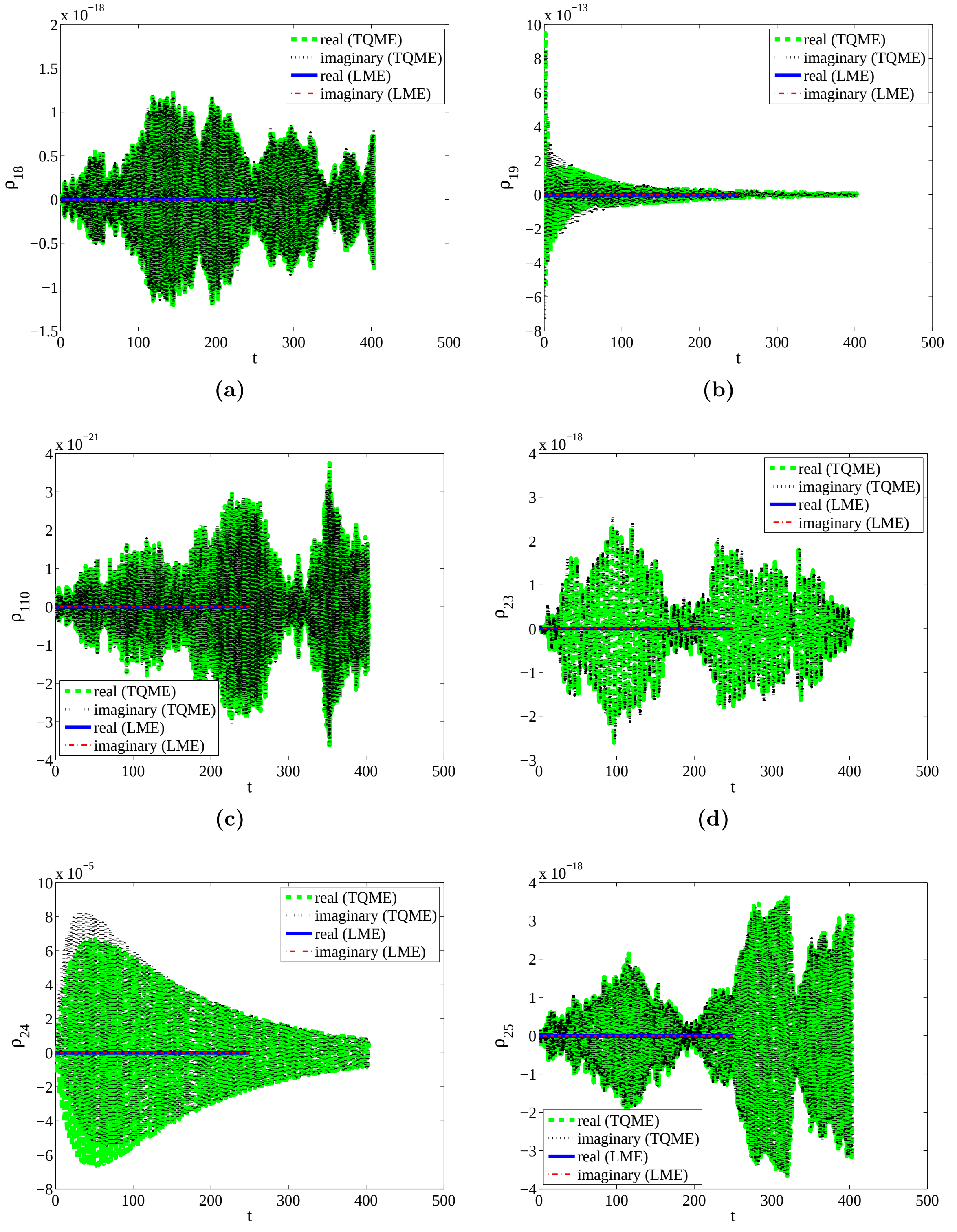
(a) (b) (c) (d) (e)

Figure 10.1.1.7: Same as 10.1.1.6 but for the diagonal density matrix elements, ρ_{66}, ρ_{77}, ρ_{88}, ρ_{99}, ρ_{1010}.



(a) (b) (c) (d) (e) (f)

Figure 10.1.1.8: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{12}, ρ_{13}, ρ_{14}, ρ_{15}, ρ_{16}, ρ_{17}.

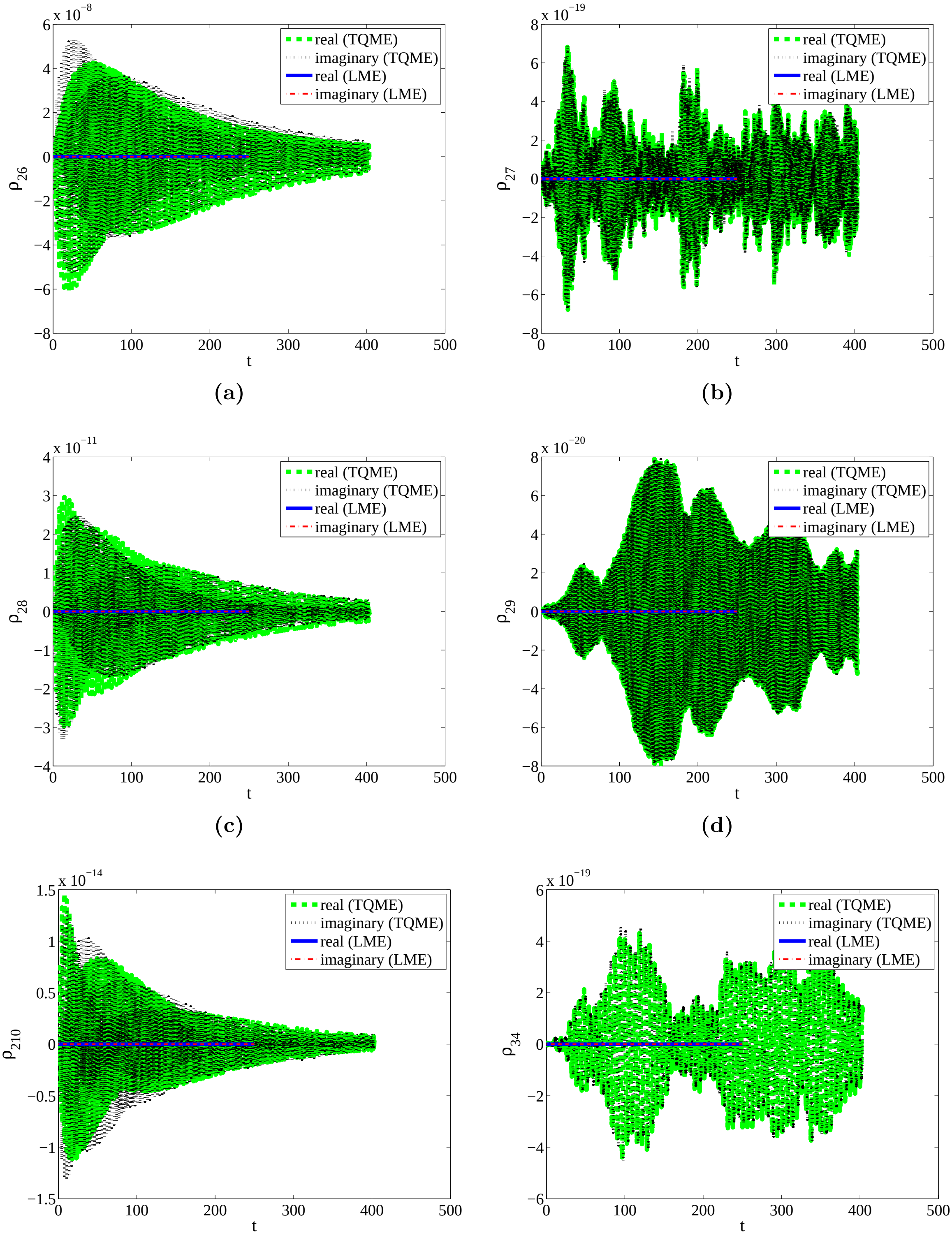


(a) (b)

(c) (d)

(e) (f)

Figure 10.1.1.9: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{18}, ρ_{19}, ρ_{110}, ρ_{23}, ρ_{24}, ρ_{25}.

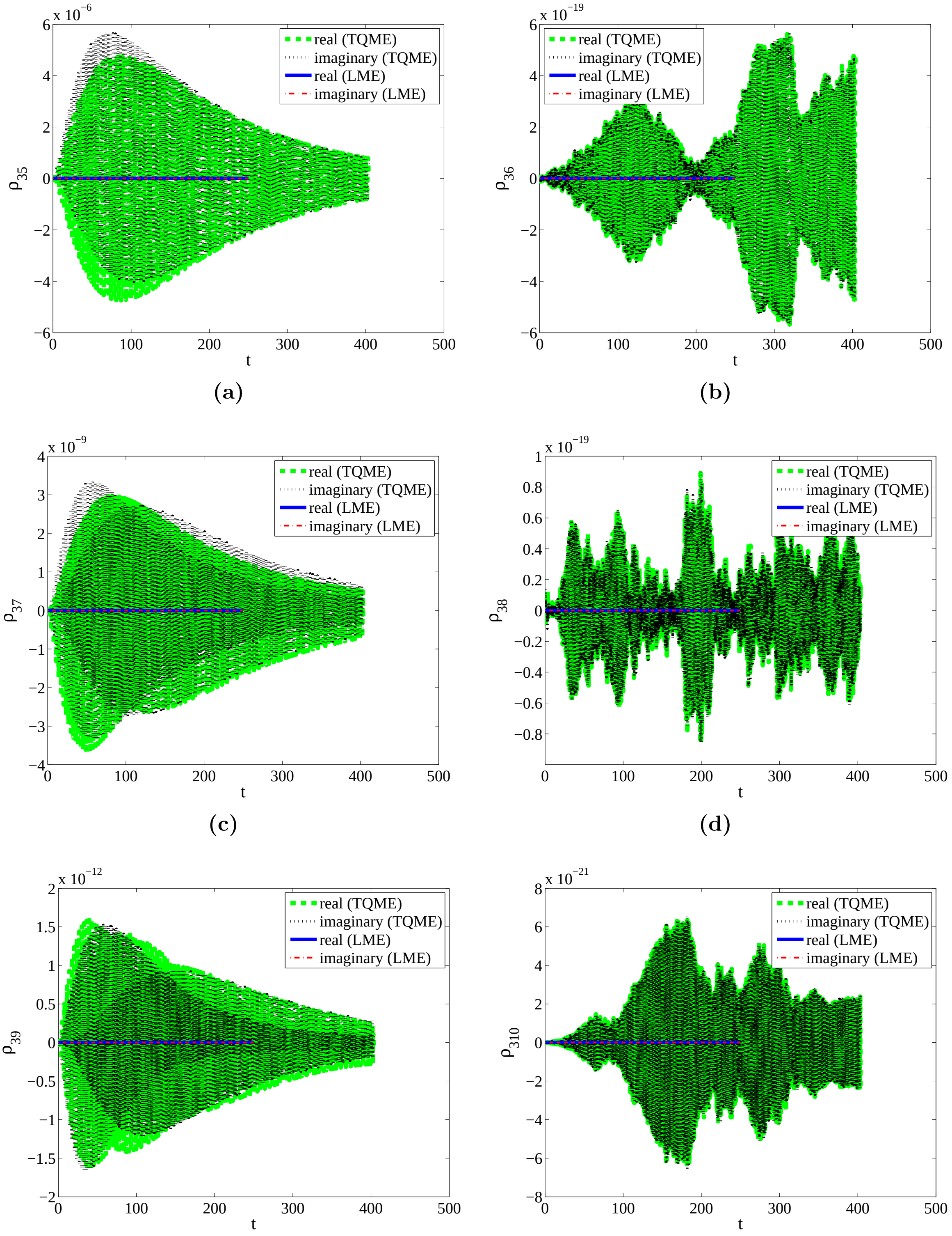


(a) (b)

(c) (d)

(e) (f)

Figure 10.1.1.10: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{26}, ρ_{27}, ρ_{28}, ρ_{29}, ρ_{210}, ρ_{34}.

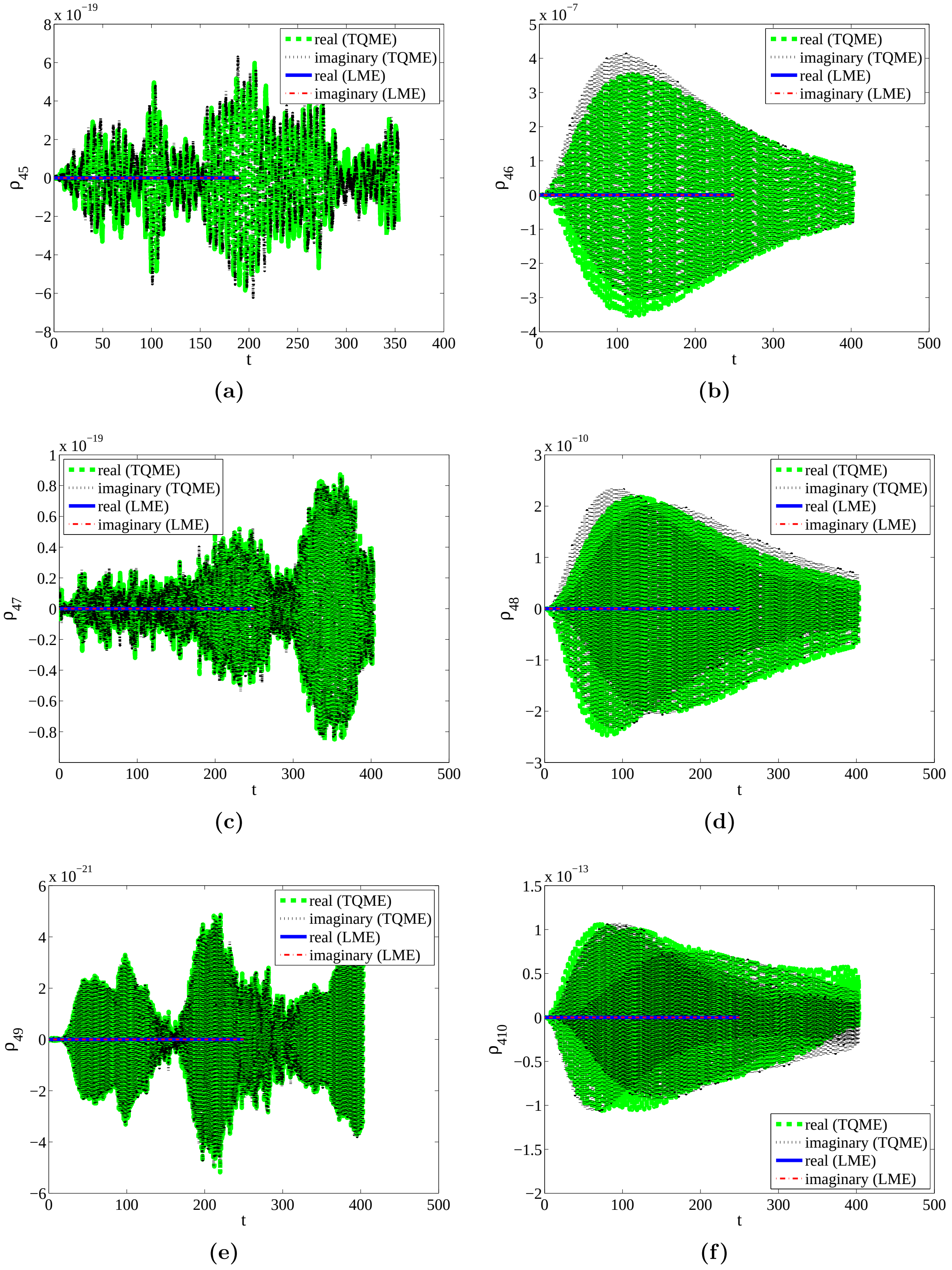


(a) **(b)**

(c) **(d)**

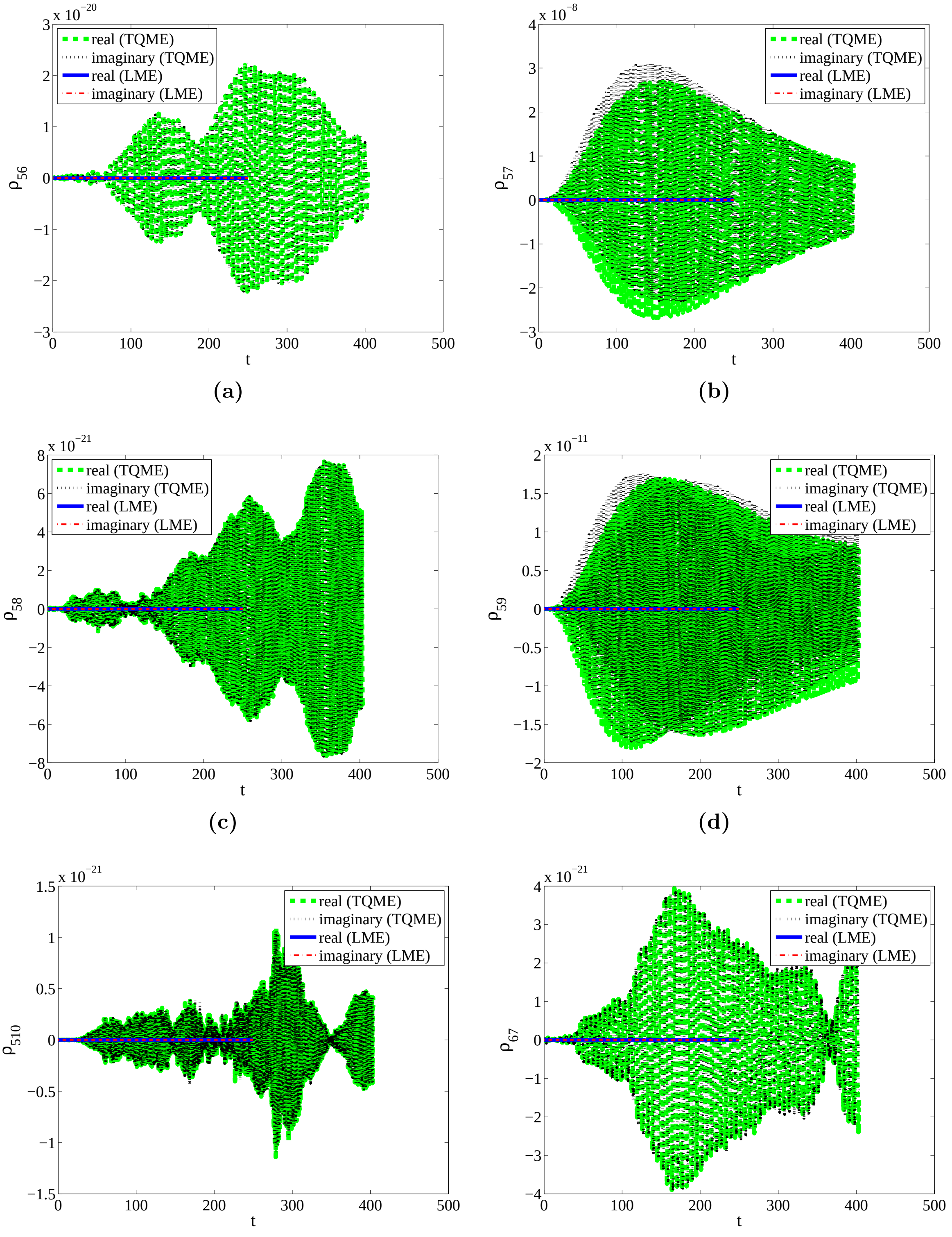
(e) **(f)**

Figure 10.1.1.11: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{35}, ρ_{36}, ρ_{37}, ρ_{38}, ρ_{39}, ρ_{310}.



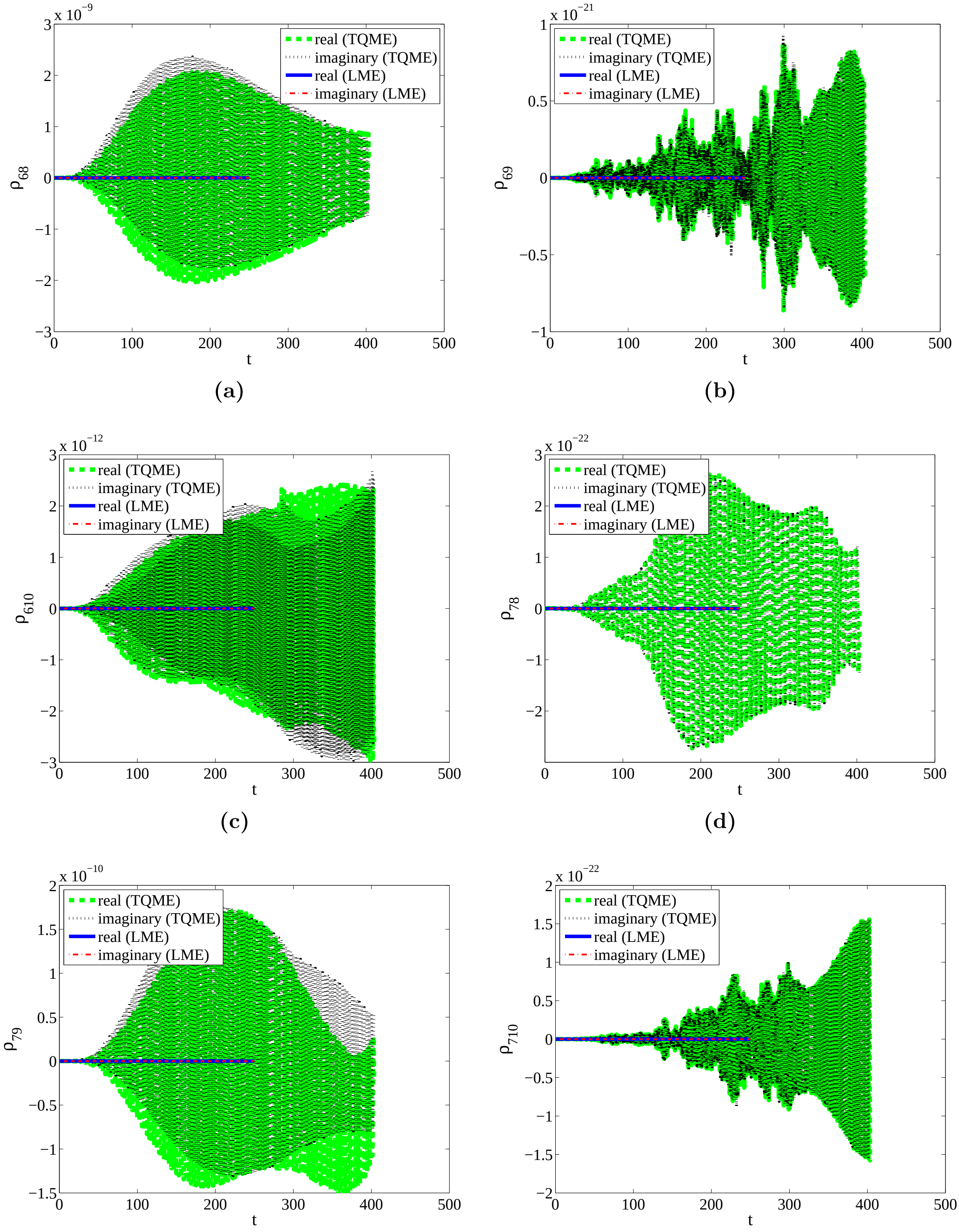
(a) (b) (c) (d) (e) (f)

Figure 10.1.1.12: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{45}, ρ_{46}, ρ_{47}, ρ_{48}, ρ_{49}, ρ_{410}.



(a) (b) (c) (d) (e) (f)

Figure 10.1.1.13: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{56}, ρ_{57}, ρ_{58}, ρ_{59}, ρ_{510}, ρ_{67}.

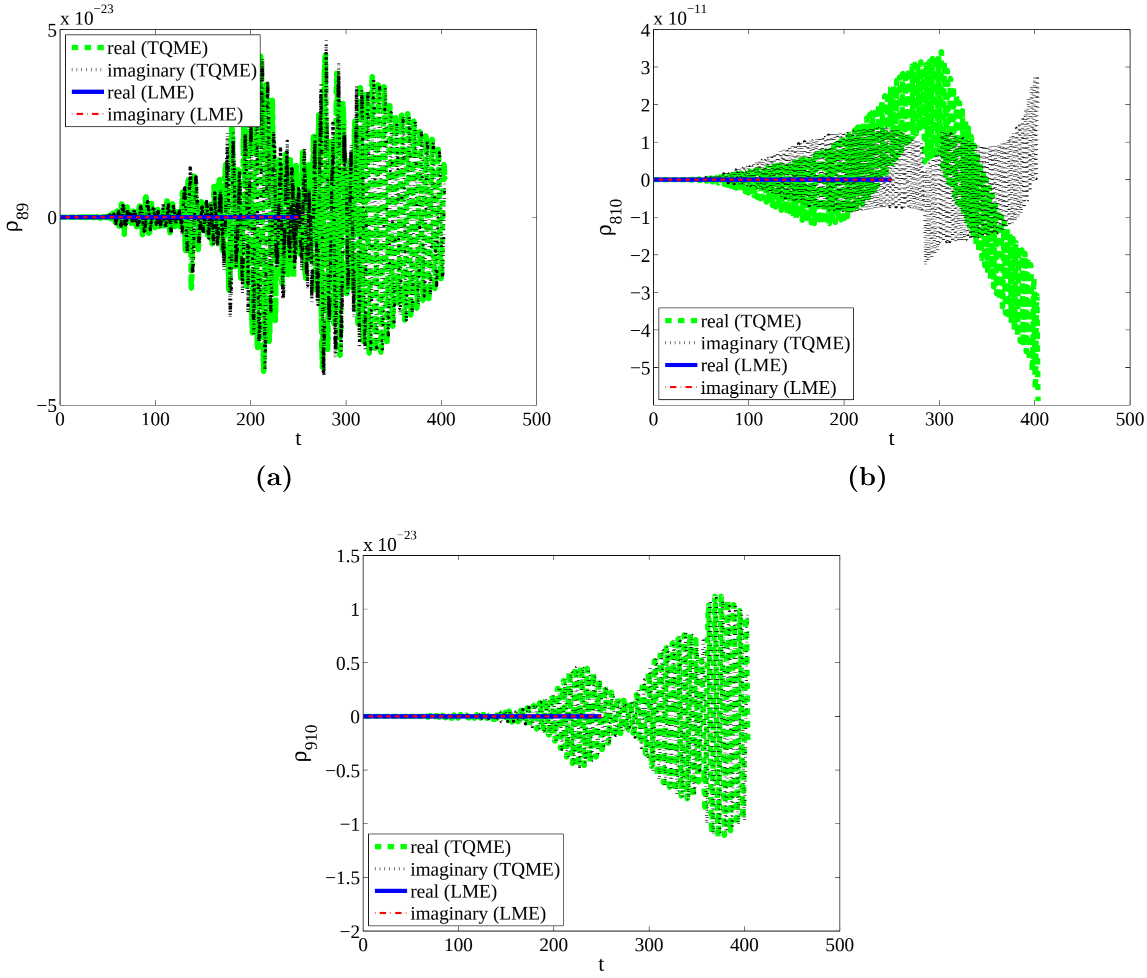


(a) (b)

(c) (d)

(e) (f)

Figure 10.1.1.14: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{68}, ρ_{69}, ρ_{610}, ρ_{78}, ρ_{79}, ρ_{710}.

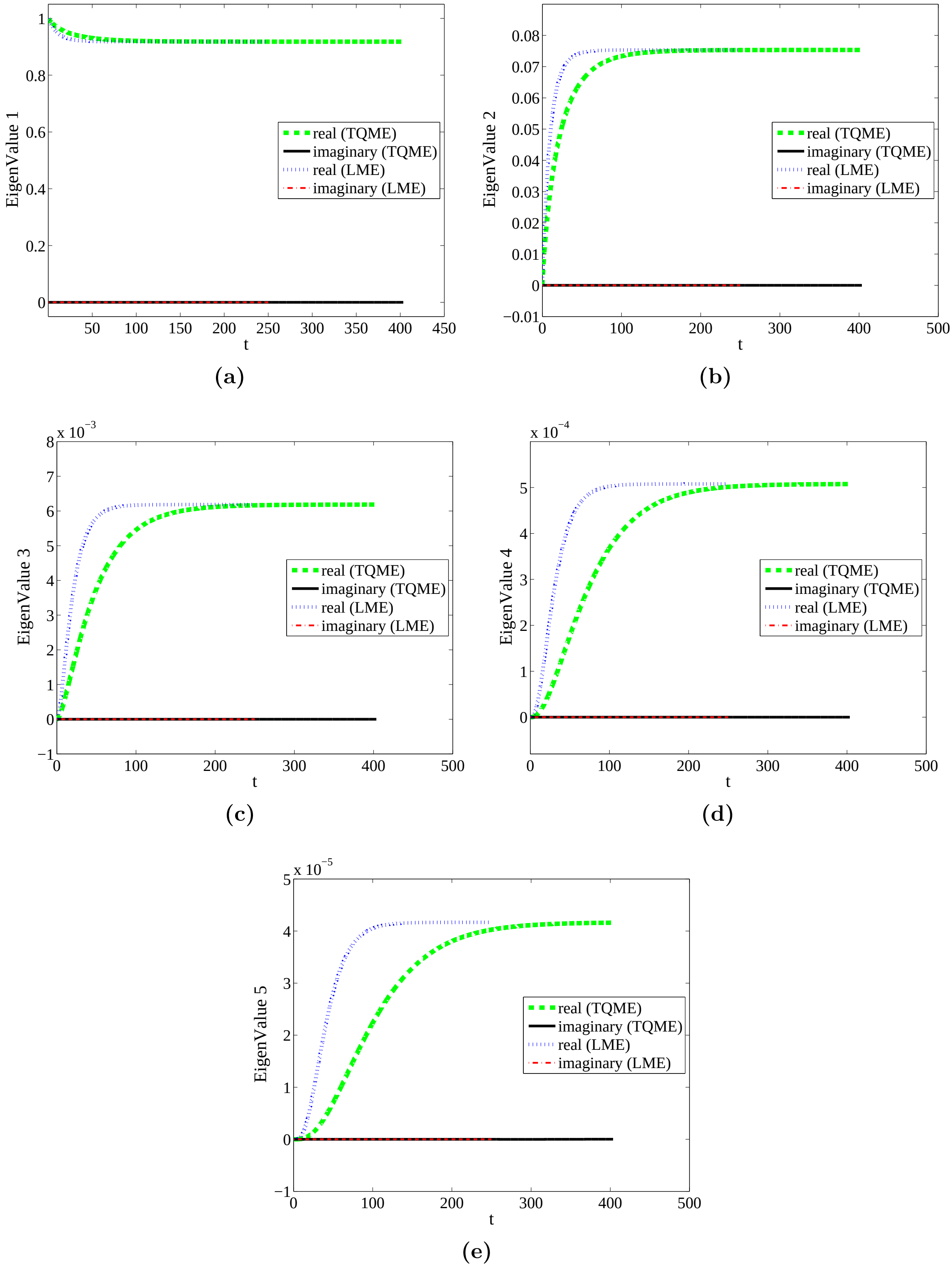


(a)

(b)

(c)

Figure 10.1.1.15: Same as 10.1.1.6 but for the non-diagonal density matrix elements, ρ_{89}, ρ_{810}, ρ_{910}.



(a)

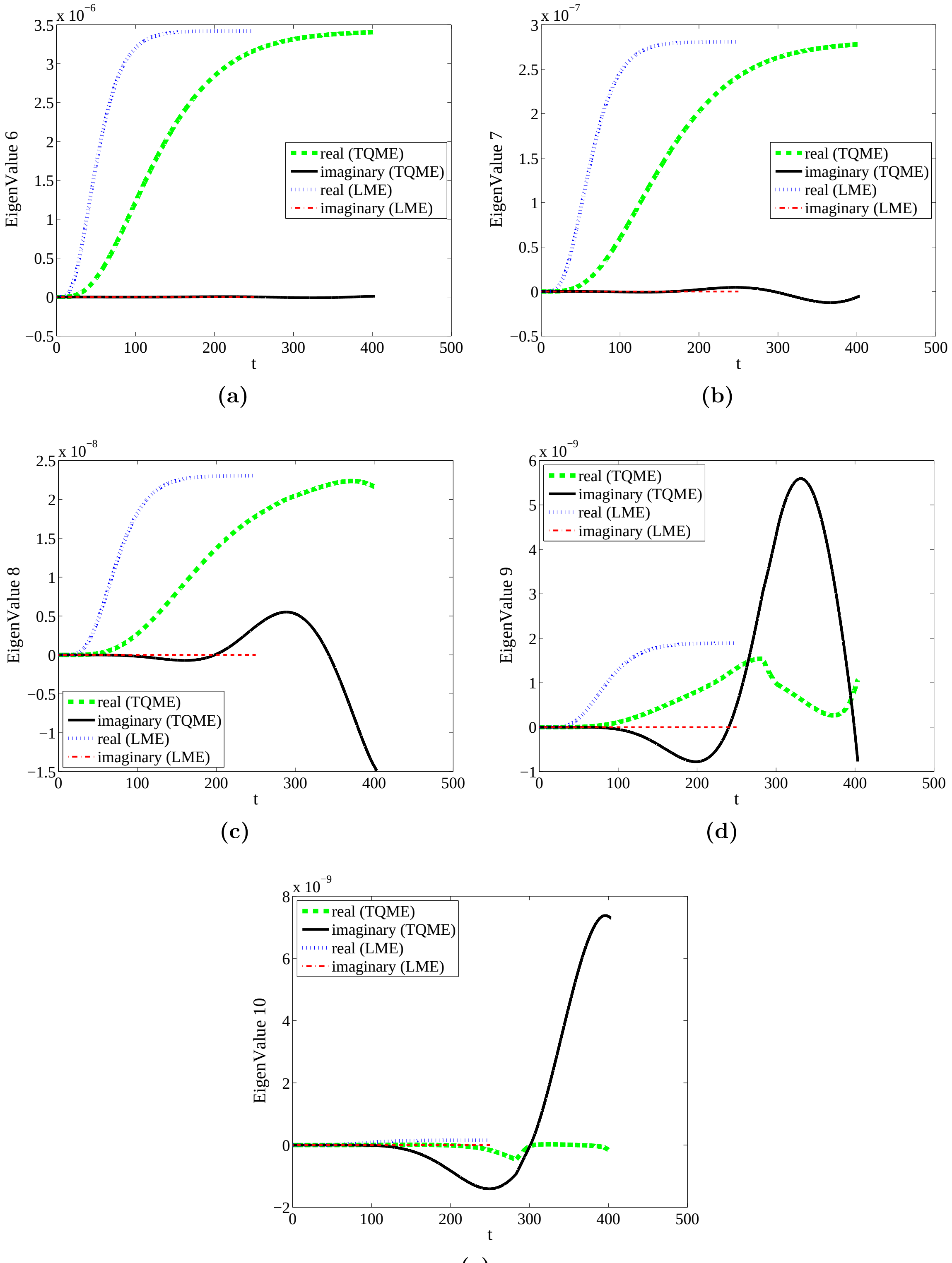
(b)

(c)

(d)

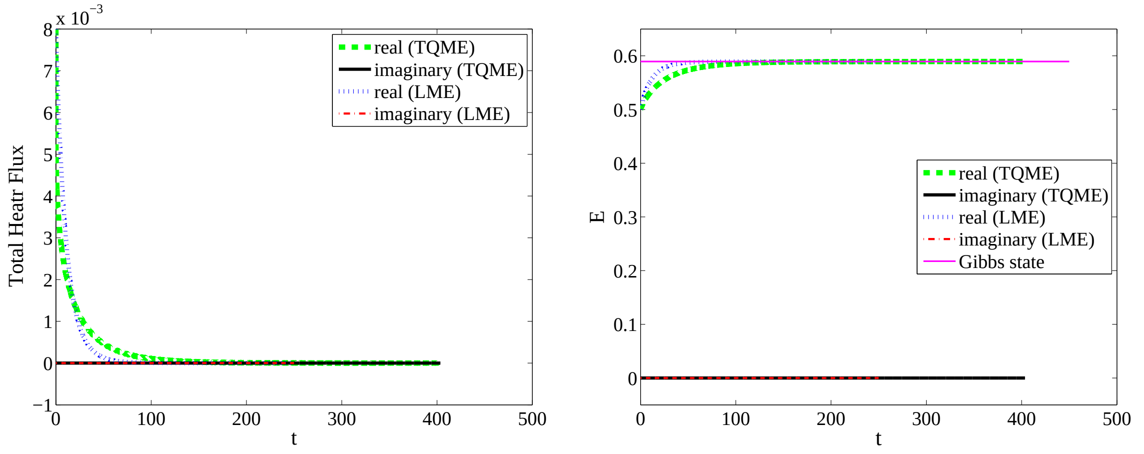
(e)

Figure 10.1.1.16: Same as 10.1.1.6 but for the first five eigenvalues of the density matrix.



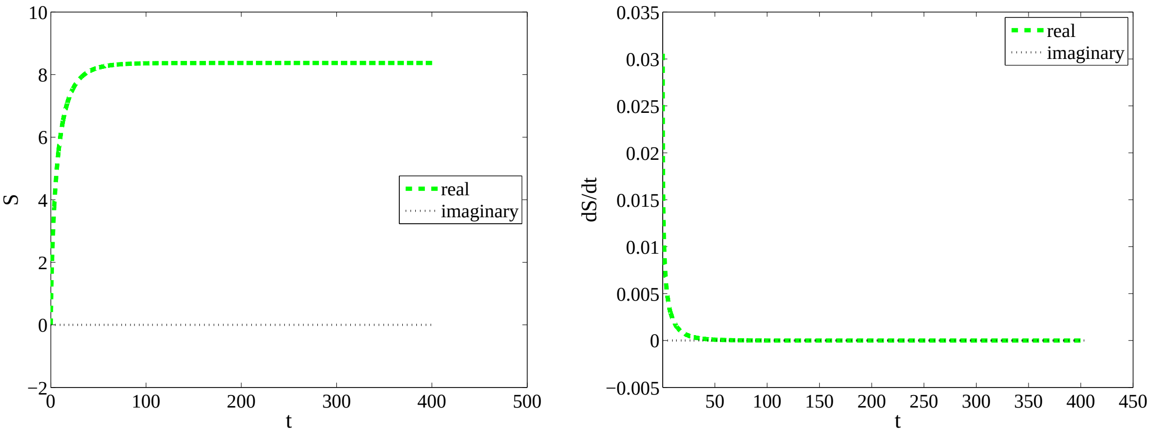
(a) **(b)** **(c)** **(d)** **(e)**

Figure 10.1.1.17: Same as 10.1.1.6 but for the last five eigenvalues of the density matrix.



(a) **(b)**

Figure 10.1.1.18: Same as 10.1.1.6 but for the heat flux of the heat bath and the energy E of the quantum system.



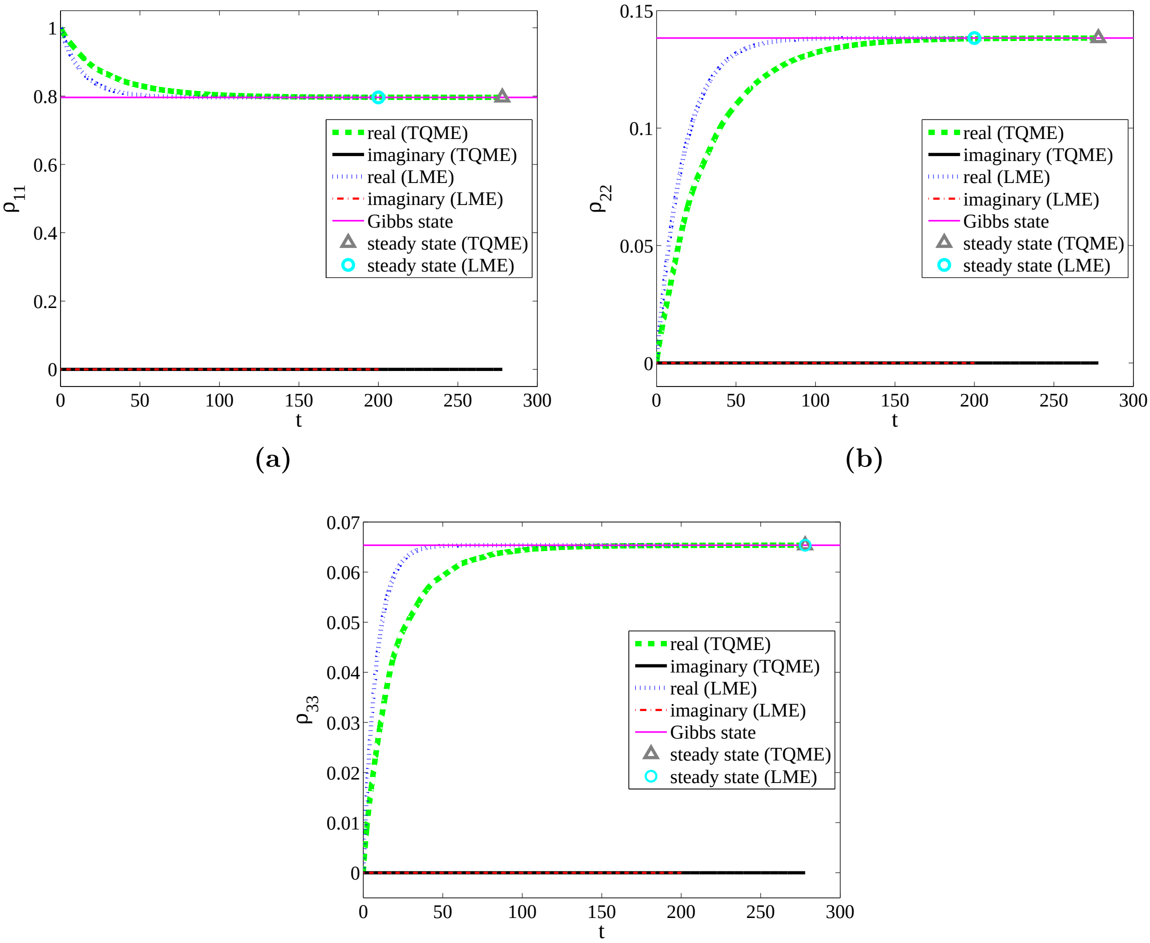
(a) **(b)**

Figure 10.1.1.19: Time evolution of the real and imaginary part of the entropy S of the system and $\frac{dS}{dt}$, using the Thermodynamic Quantum Master Equation (TQME) (real (green), imaginary (black)) for the case of the Harmonic Oscillator (10 states), with $T_e = 0.4$ and $\gamma = 0.01$.

10.1.2 Direct Steady-State Solution

In this section, we present the results obtained by an independent, non-linear matrix algebra solver that we implemented for computing the steady-state solution of the density matrix. These steady-state solutions are compared with the corresponding values taken from the dynamic relaxation of numerical integration for all the studied occasions.

Three-Level System (Qutrit)



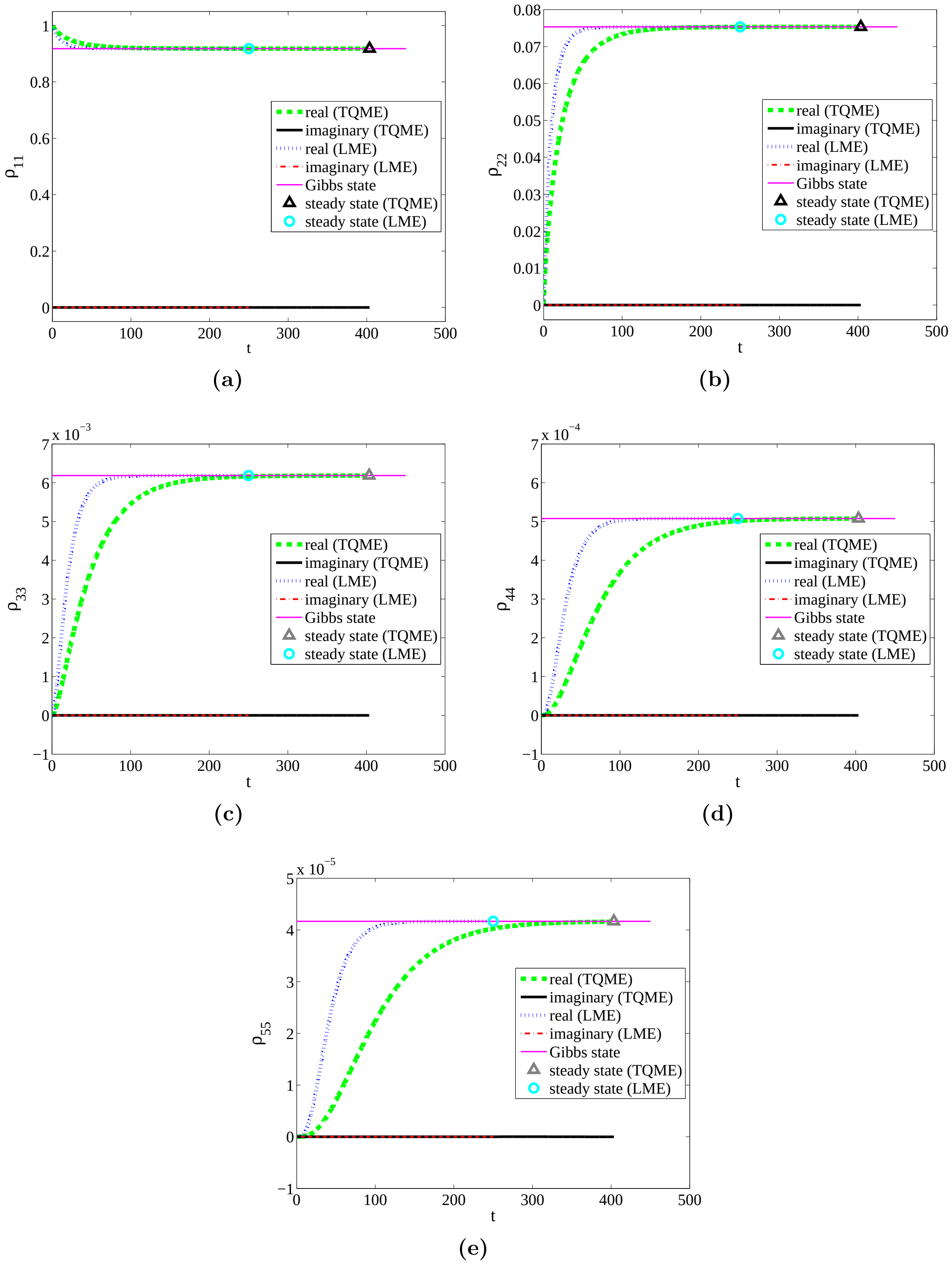
(a)

(b)

(c)

Figure 10.1.2.1: Comparison of the steady-state solution of the diagonal density matrix elements, $\rho_{11}, \rho_{22}, \rho_{33}$, between the time integration and the direct calculation of the steady-state values, using the Lindblad Master Equation (LME) (time integration: real (green), imaginary (black), steady-state solution: real (grey triangular)) and the Thermodynamic Quantum Master Equation (TQME) (time integration: real (blue), imaginary (red), steady-state solution: real (light blue circle)), in the case of the Three-Level system (Qutrit), with $T_e = 0.4$ and $\gamma = 0.01$.

Harmonic Oscillator (10 states)



(a)

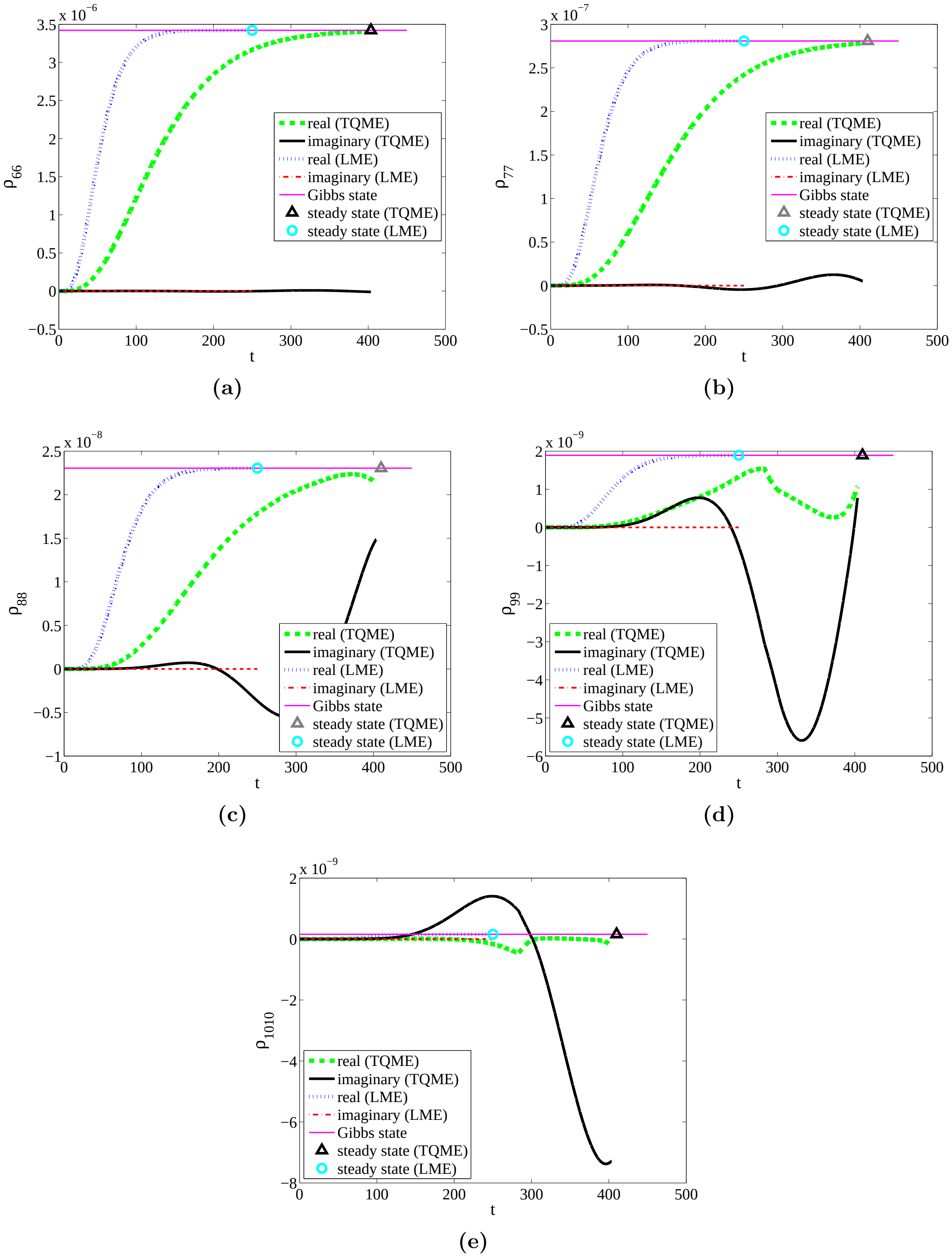
(b)

(c)

(d)

(e)

Figure 10.1.2.2: Comparison of the steady-state solution of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, ρ_{44}, ρ_{55}, between the time integration and the direct calculation of the steady-state values, using the Lindblad Master Equation (LME) (time integration: real (green), imaginary (black), steady-state solution: real (grey triangular)) and the Thermodynamic Quantum Master Equation (TQME) (time integration: real (blue), imaginary (red), steady-state solution: real (light blue circle)), in the case of the Harmonic Oscillator (10 states), with $T_e = 0.4$ and $\gamma = 0.01$.



(a) (b) (c) (d) (e)

Figure 10.1.2.3: Same as 10.1.2.2 but for ρ_{66}, ρ_{77}, ρ_{88}, ρ_{99}, ρ_{1010}.

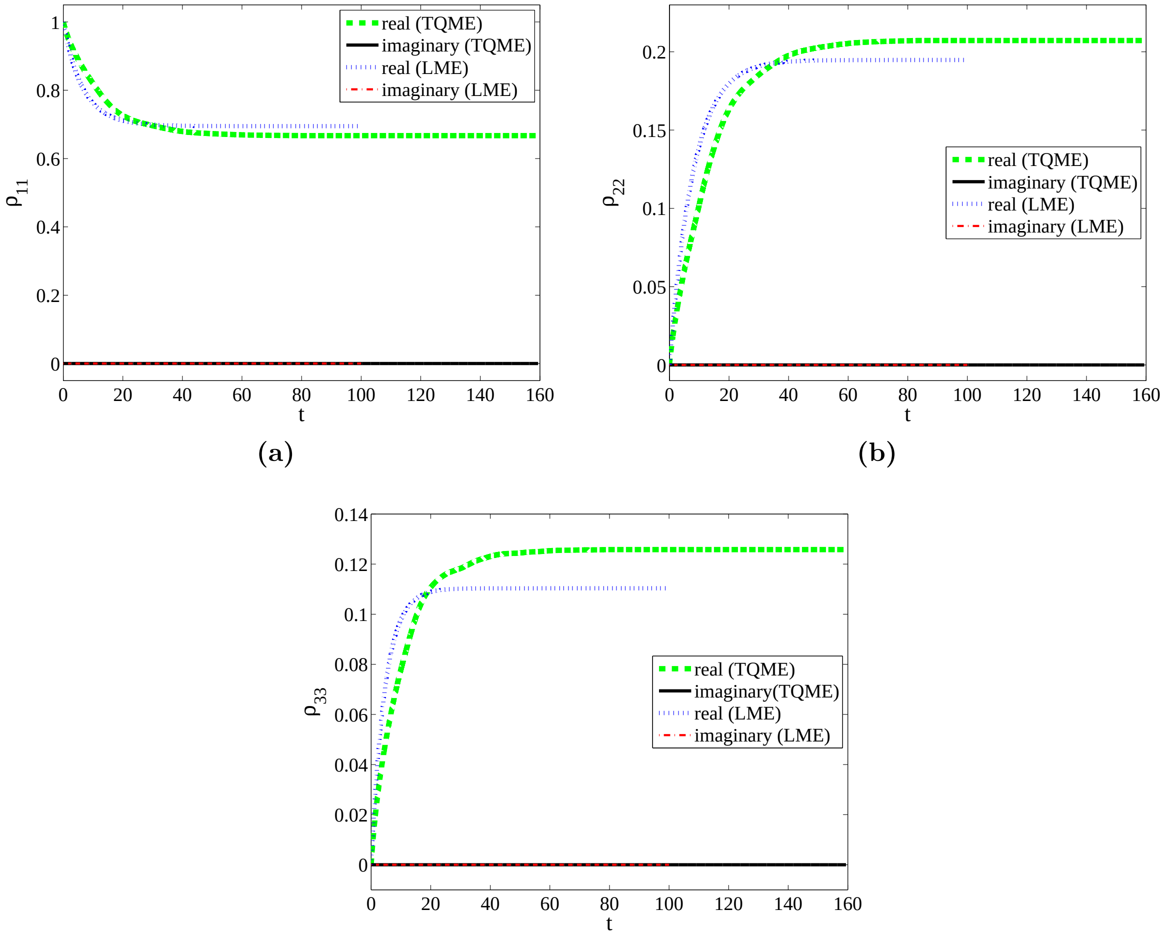
10.2 Quantum Susbsystem coupled to Two Heat Baths - 1^{st} Set

In this section, results are presented that have been obtained through the time integration and the direct calculation of the steady-state values using the Lindblad Master Equation (LME), Eq. 7.1.2, and the Thermodynamic Quantum Master Equation (TQME), Eq. 7.2.4.1. These results refer to the two cases that we study; the three-level and the harmonic oscillator as quantum subsystems coupled to two heat baths. The inputs where the same mentioned in section 9.2, with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

10.2.1 Time Integration

The integration scheme used in this work is the Adams-Bashforth 4th order ($s = 4$) in Eq. 8.1.4) with the help of single-step Euler's scheme in order to obtain the four starting values. The integration time step that we set was $h = 10^{-2}$.

Three-Level System (Qutrit)

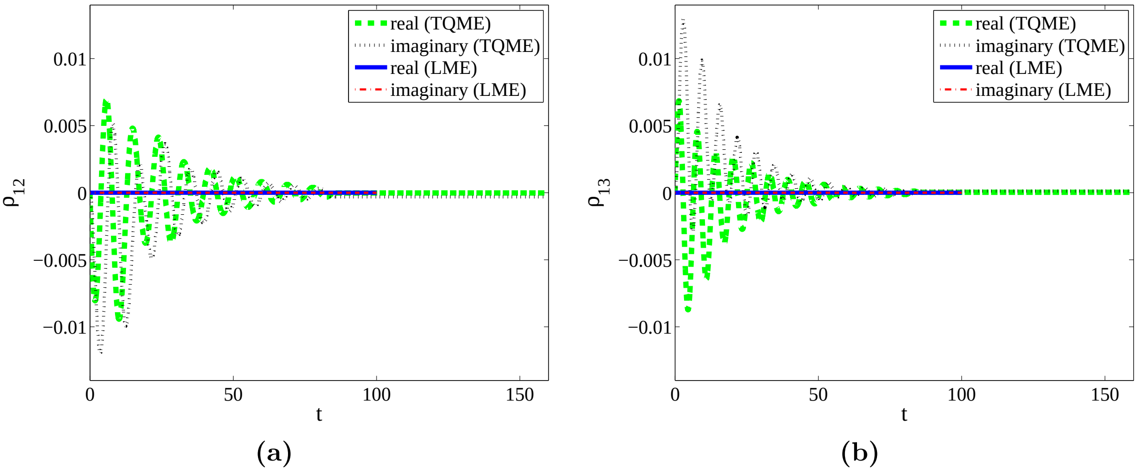


(a)

(b)

(c)

Figure 10.2.1.1: Time evolution of the real and imaginary part of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, using the Lindblad Master Equation (LME) (real (green), imaginary (black)) and the Thermodynamic Quantum Master Equation (TQME) (real (blue), imaginary (red)) for the case of the Three-Level system (Qutrit), with $T_{e,l}$ = 0.4, $T_{e,r}$ = 0.8 and γ_l = γ_r = 0.01.



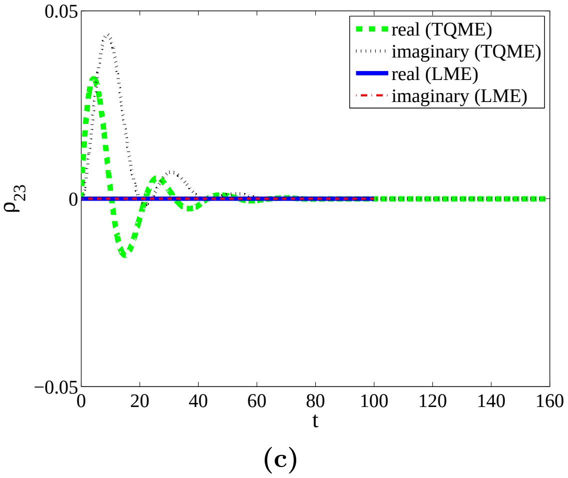
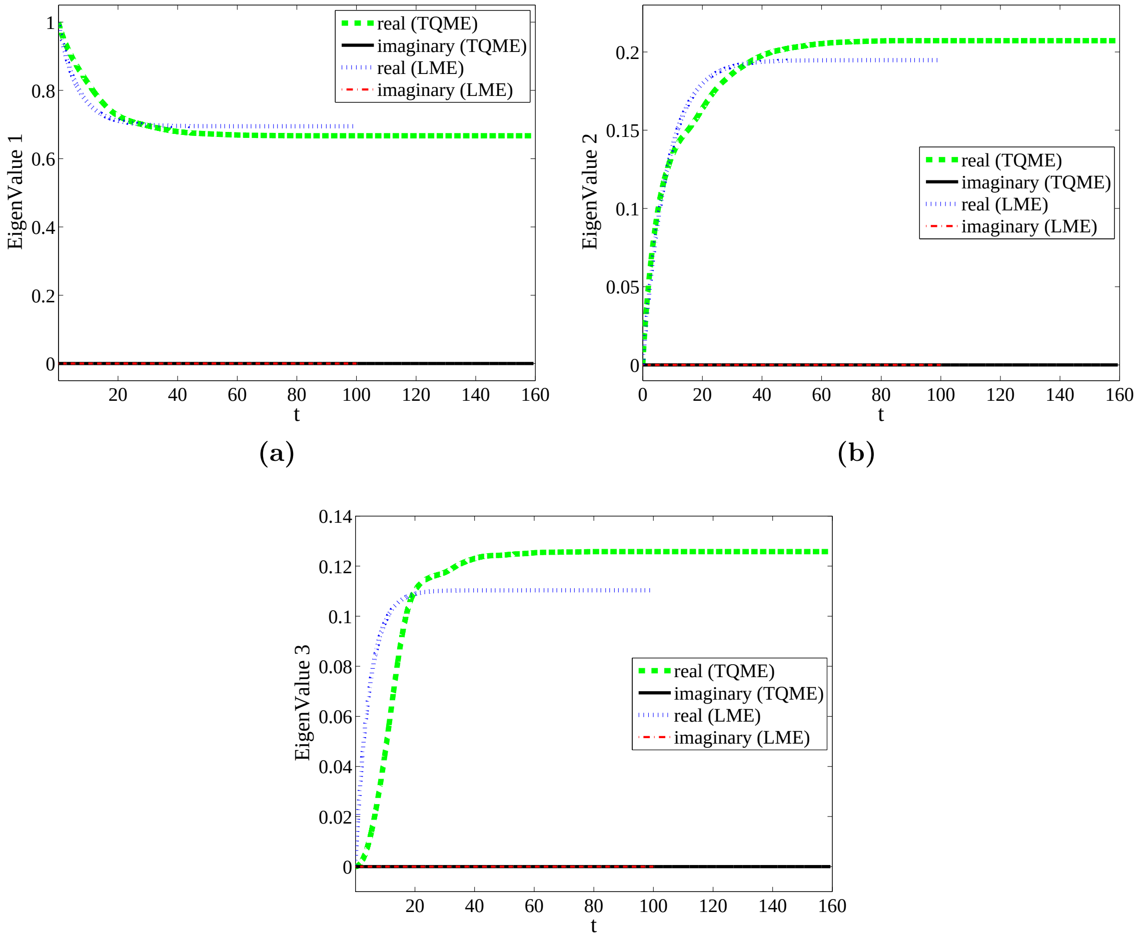


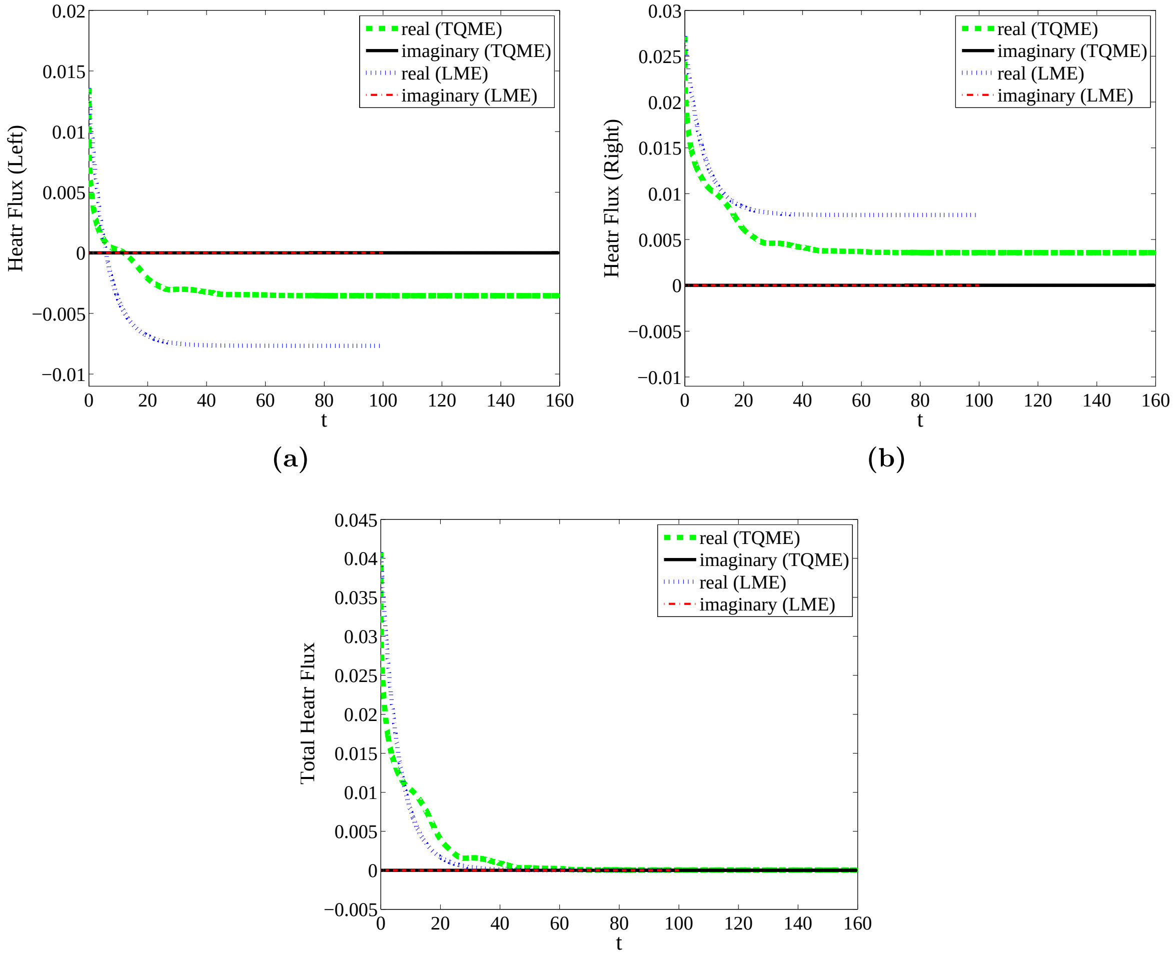
Figure 10.2.1.2: Same as 10.2.1.1 but for the non-diagonal density matrix elements, ρ_{12}, ρ_{13}, ρ_{23}.



(a) **(b)**

(c)

Figure 10.2.1.3: Same as 10.2.1.1 but for the eigenvalues of the density matrix.



(a) (b)

(c)

Figure 10.2.1.4: Same as 10.2.1.1 but for the heat flux of the left (10.2.1.4a), right (10.2.1.4b) heat baths and the total one (10.2.1.4c).

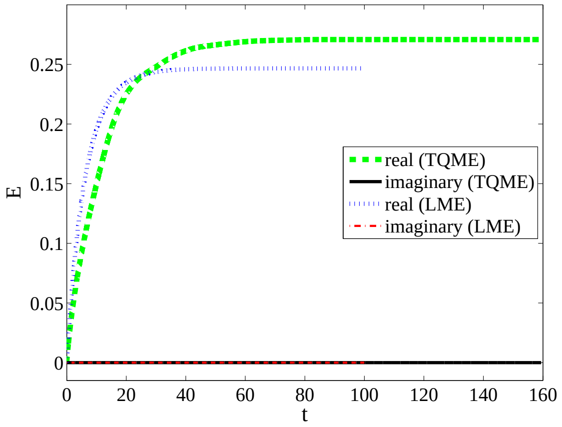
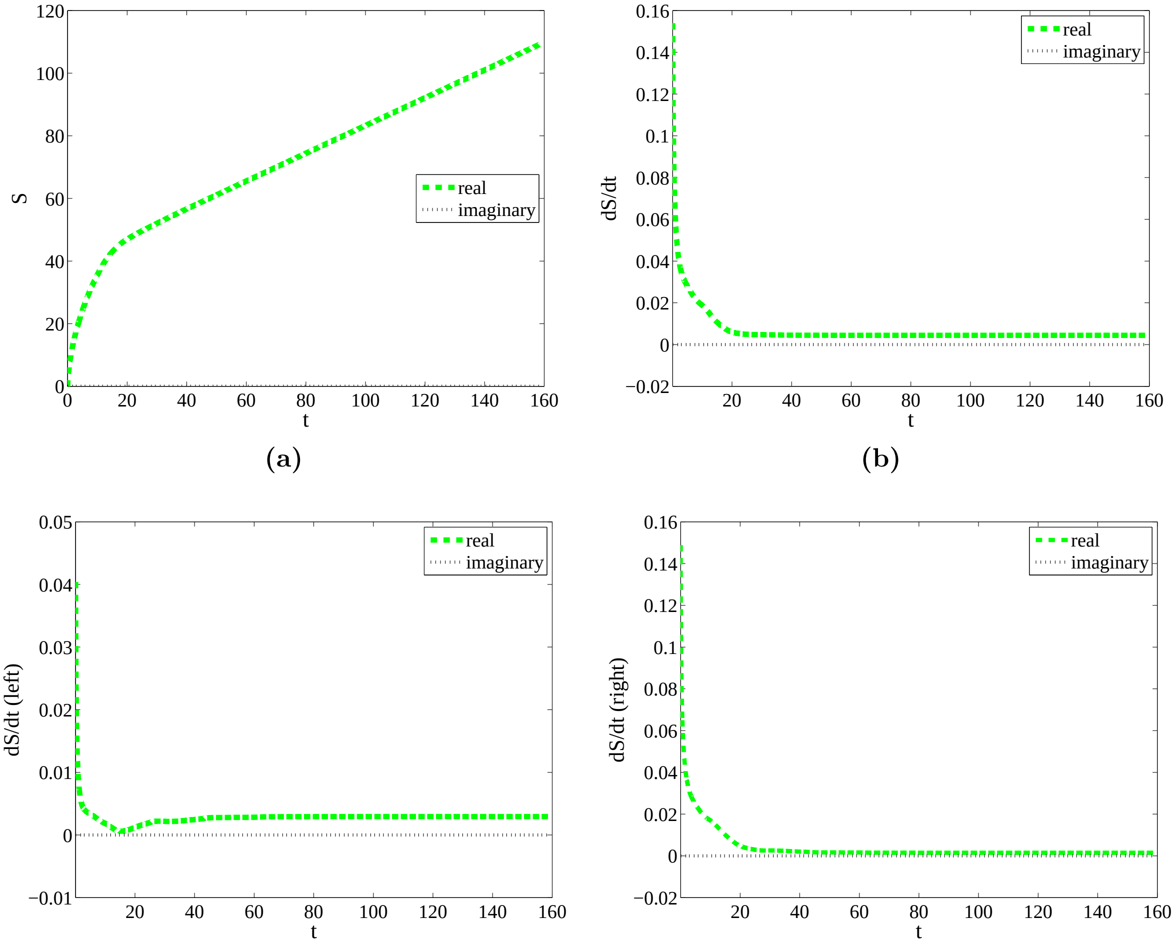


Figure 10.2.1.5: Same as 10.2.1.1 but for the energy E of the system.

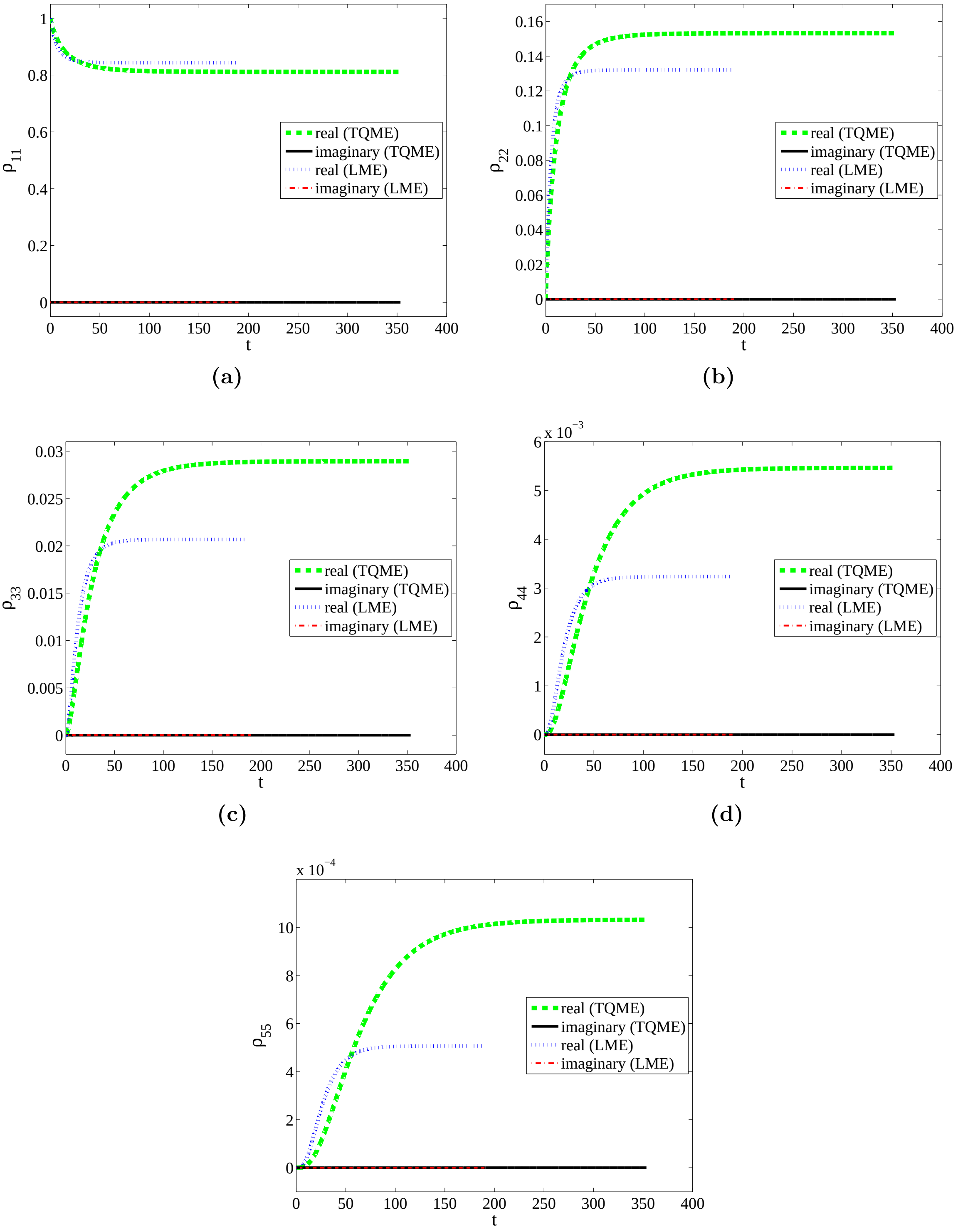


(a) **(b)**

(c) **(d)**

Figure 10.2.1.6: Time evolution of the real and imaginary part of the entropy S of the system and $\frac{dS}{dt}$, $\frac{dS}{dt}$ (left), $\frac{dS}{dt}$ (right), using the Thermodynamic Quantum Master Equation (TQME) (real (green), imaginary (black)) for the case of the Three-Level system (Qutrit), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

Harmonic Oscillator (10 states)



(a)

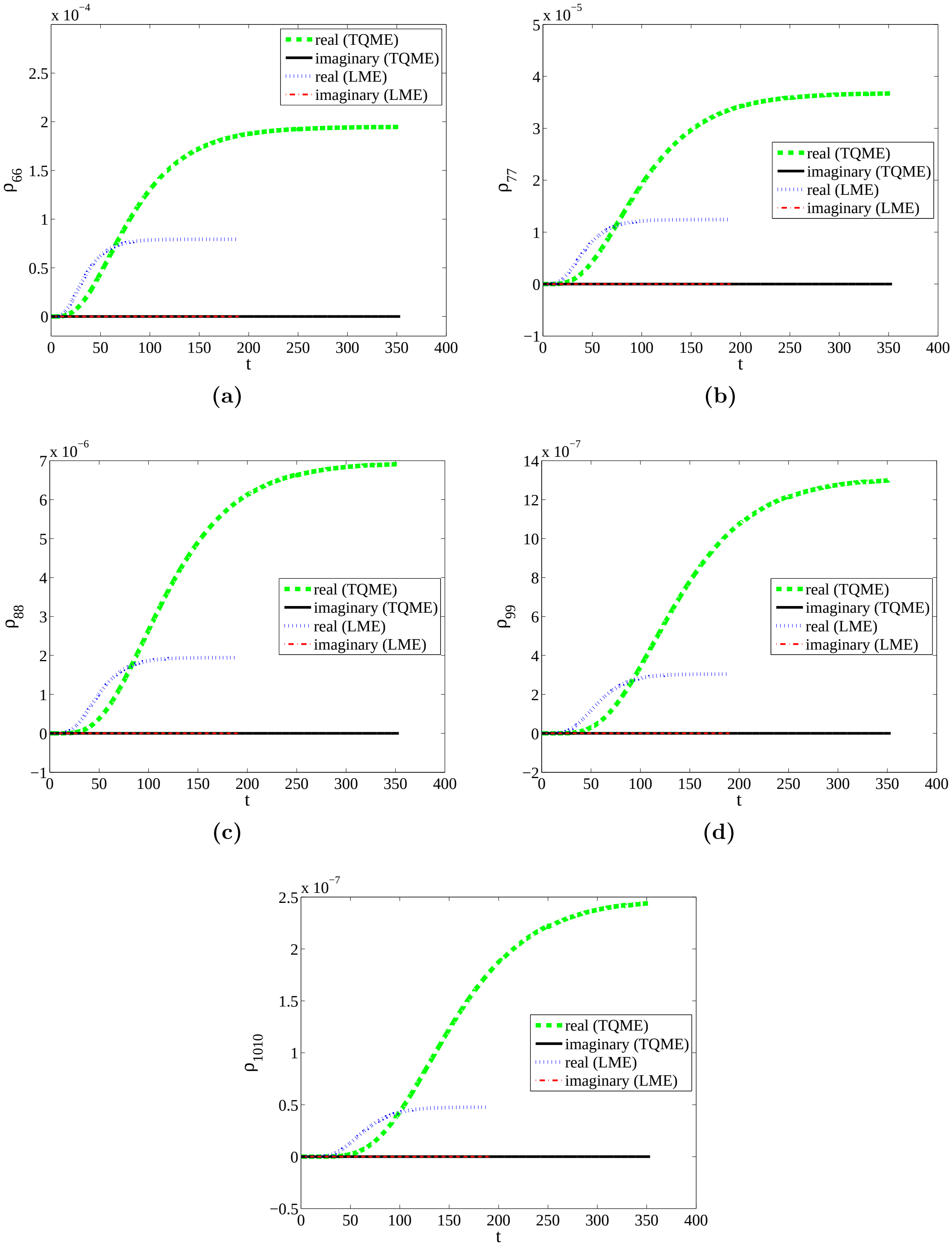
(b)

(c)

(d)

(e)

Figure 10.2.1.7: Time evolution of the real and imaginary part of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, using the Lindblad Master Equation (LME) (real (green), imaginary (black)) and the Thermodynamic Quantum Master Equation (TQME) (real (blue), imaginary (red)) for the case of the Harmonic Oscillator (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.01$.



(a)

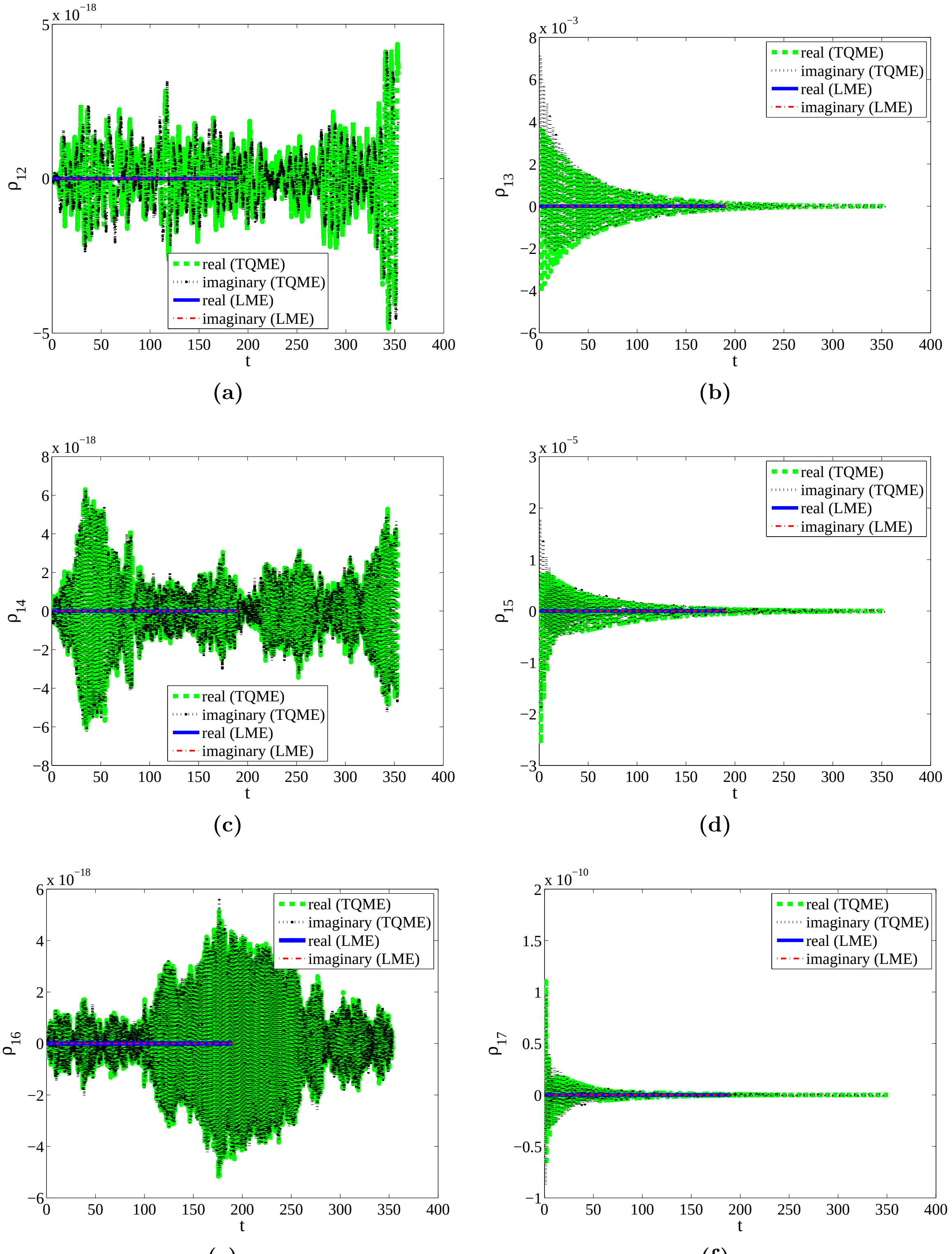
(b)

(c)

(d)

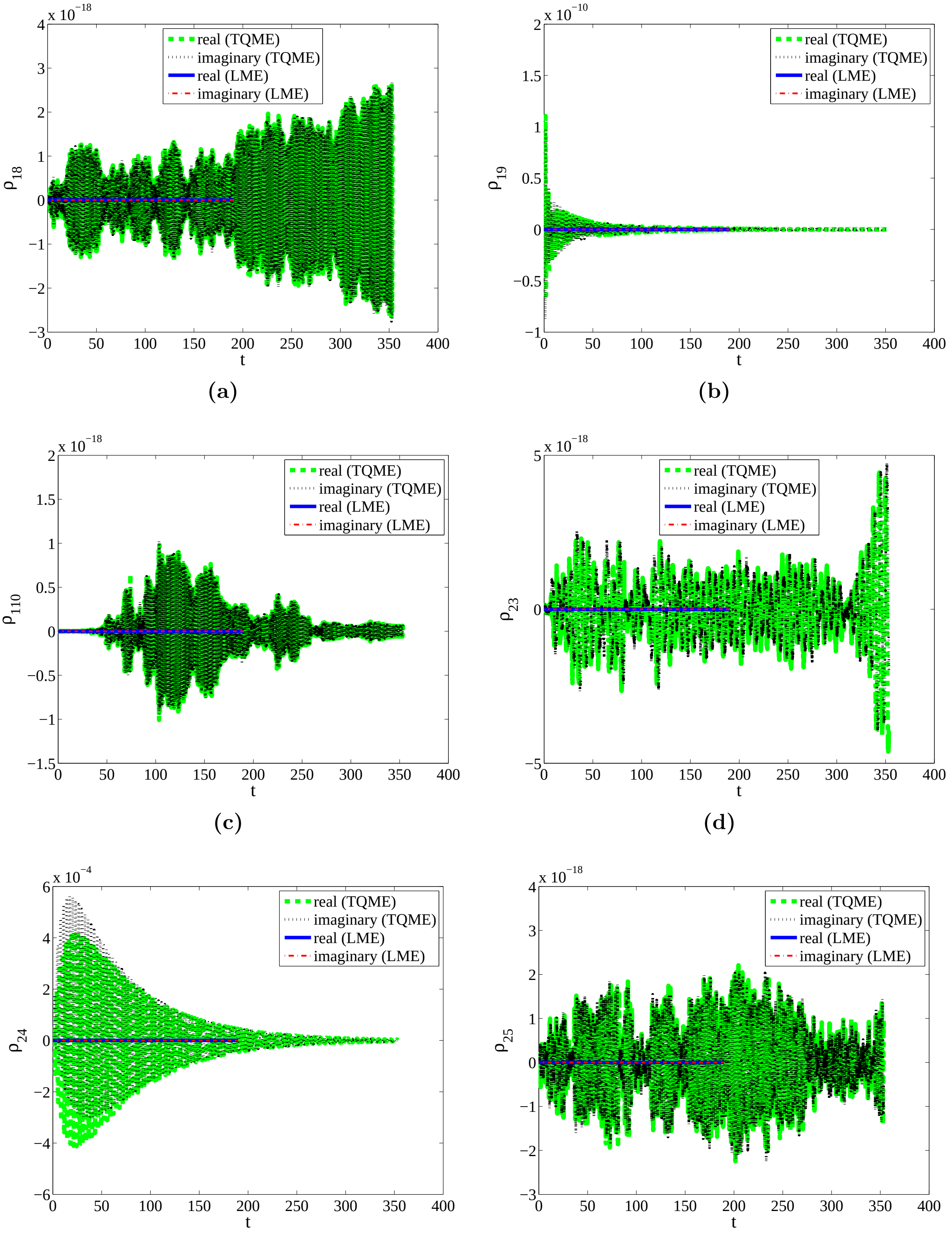
(e)

Figure 10.2.1.8: Same as 10.2.1.7 but for the diagonal density matrix elements, ρ_{66}, ρ_{77}, ρ_{88}, ρ_{99}, ρ_{1010}.



(a) (b) (c) (d) (e) (f)

Figure 10.2.1.9: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{12}, ρ_{13}, ρ_{14}, ρ_{15}, ρ_{16}, ρ_{17}.

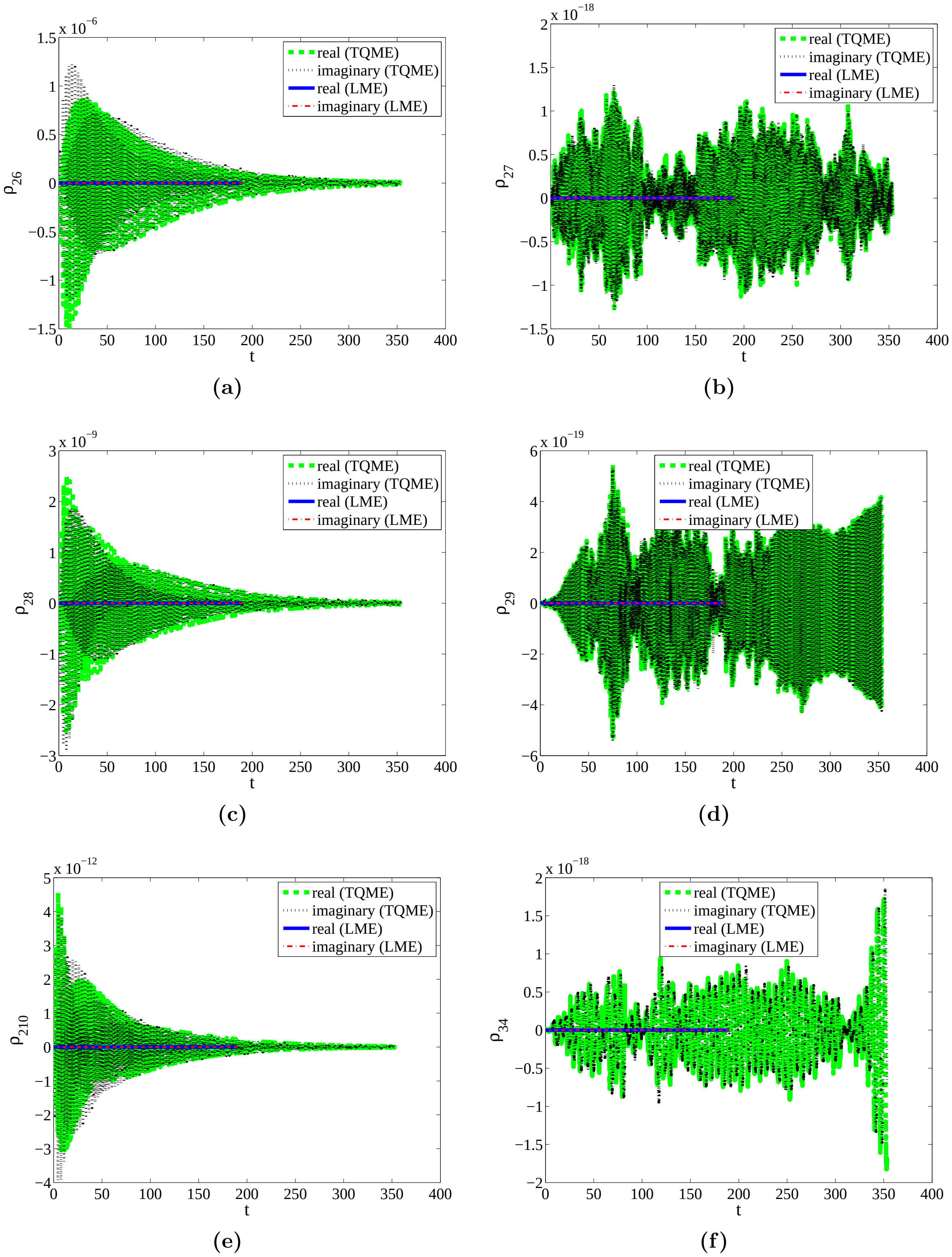


(a) **(b)**

(c) **(d)**

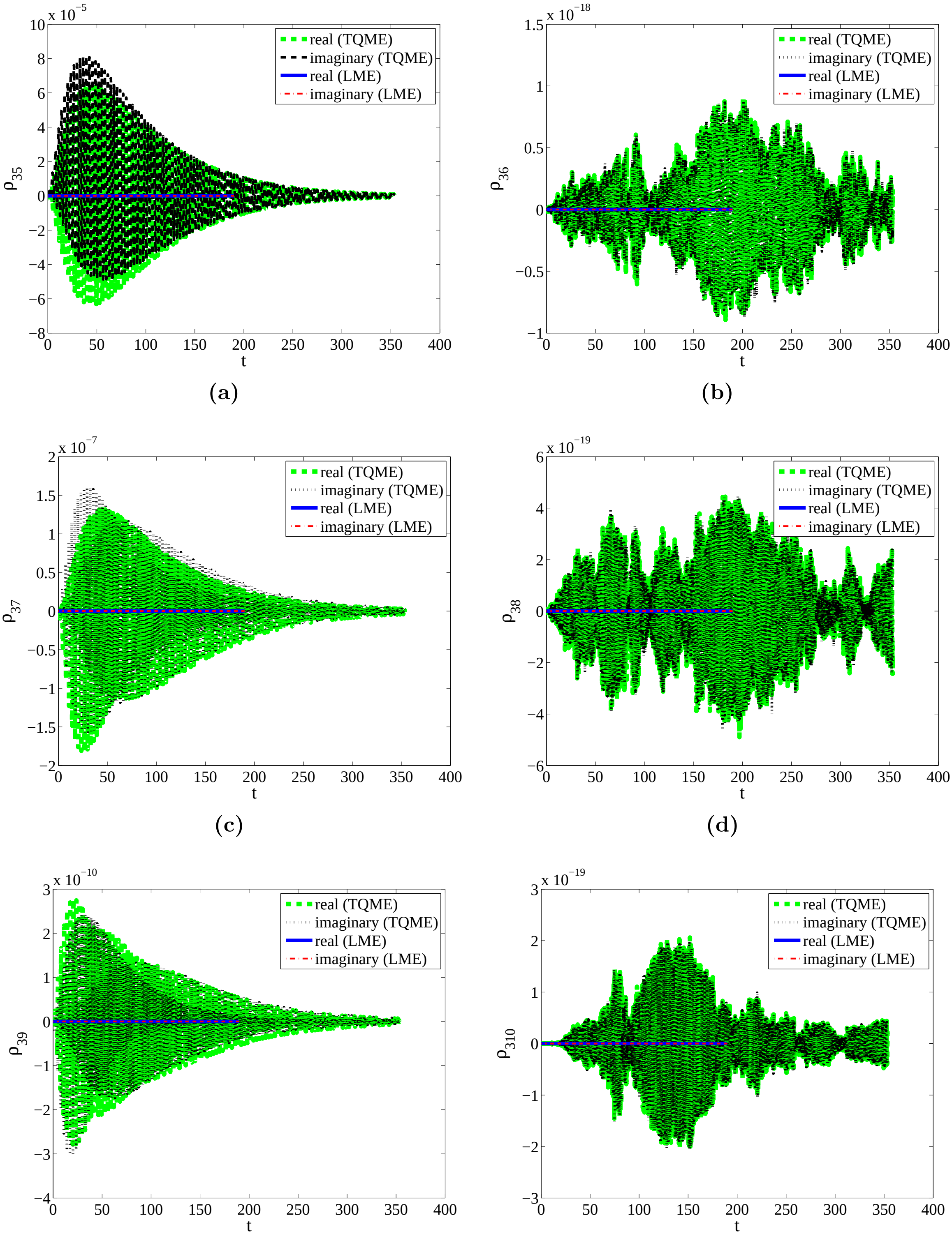
(e) **(f)**

Figure 10.2.1.10: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{18}, ρ_{19}, ρ_{110}, ρ_{23}, ρ_{24}, ρ_{25}.



(a) (b) (c) (d) (e) (f)

Figure 10.2.1.11: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{26}, ρ_{27}, ρ_{28}, ρ_{29}, ρ_{210}, ρ_{34}.

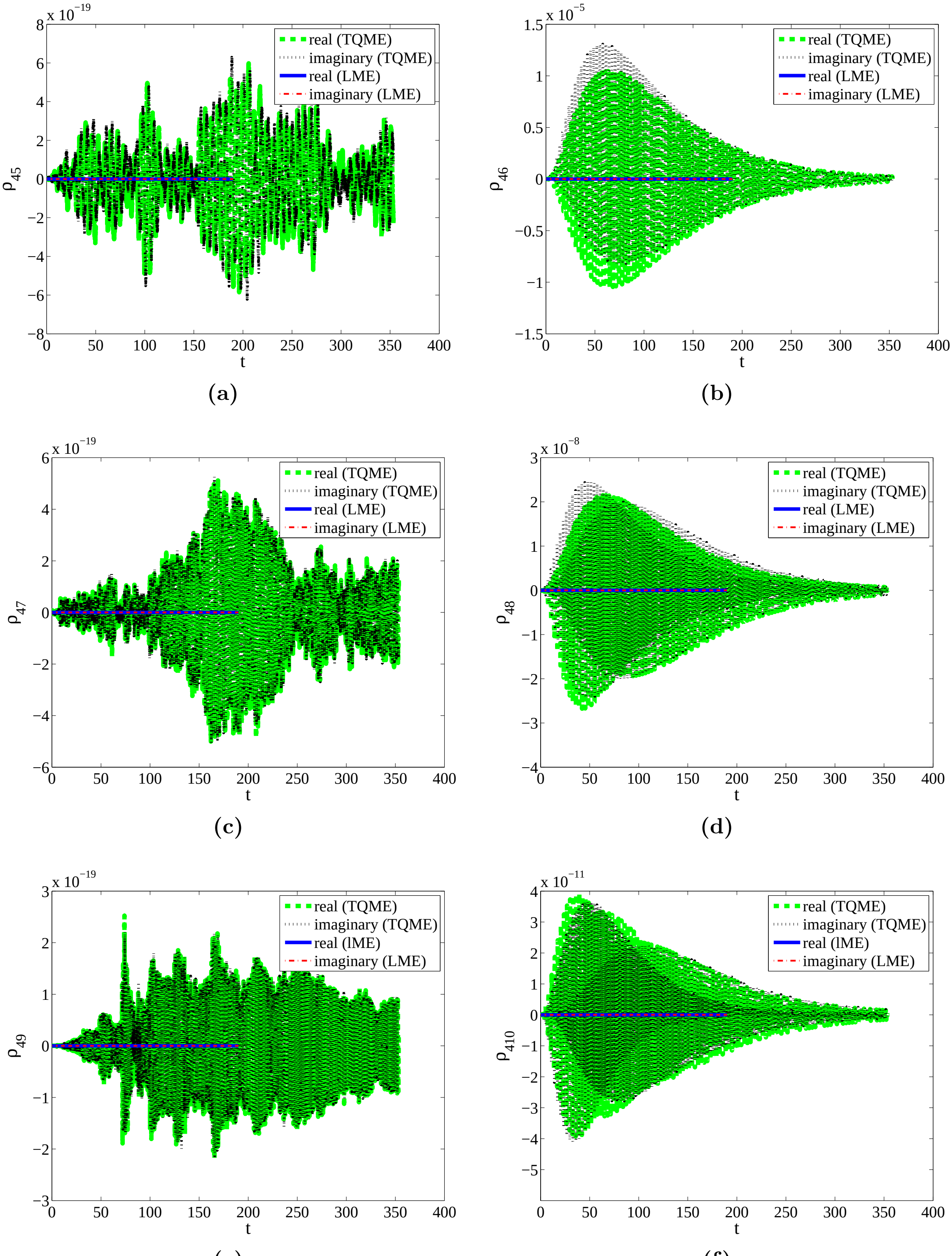


(a) (b)

(c) (d)

(e) (f)

Figure 10.2.1.12: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{35}, ρ_{36}, ρ_{37}, ρ_{38}, ρ_{39}, ρ_{310}.

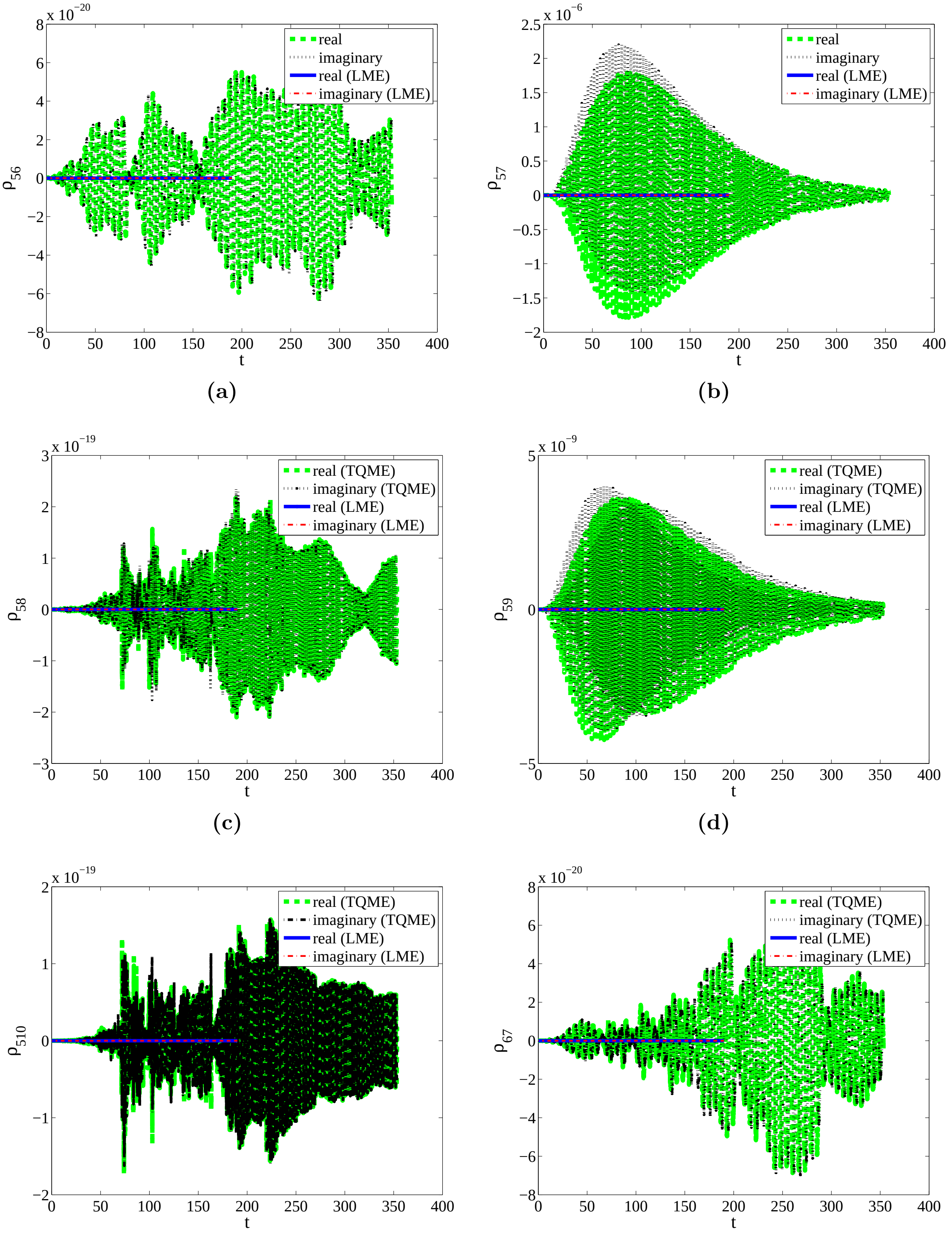


(a) **(b)**

(c) **(d)**

(e) **(f)**

Figure 10.2.1.13: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{45}, ρ_{46}, ρ_{47}, ρ_{48}, ρ_{49}, ρ_{410}.

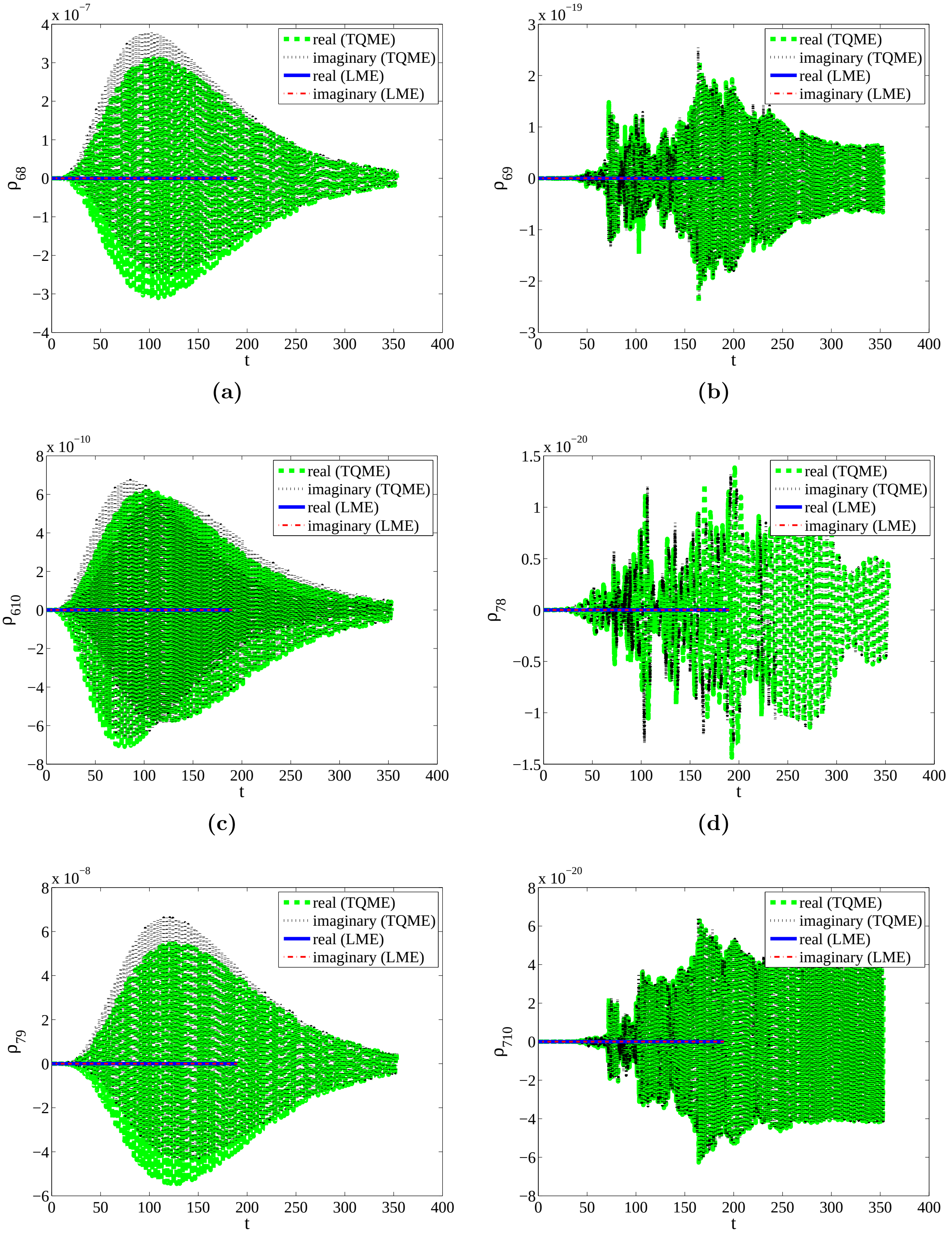


(a) **(b)**

(c) **(d)**

(e) **(f)**

Figure 10.2.1.14: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{56}, ρ_{57}, ρ_{58}, ρ_{59}, ρ_{510}, ρ_{67}.

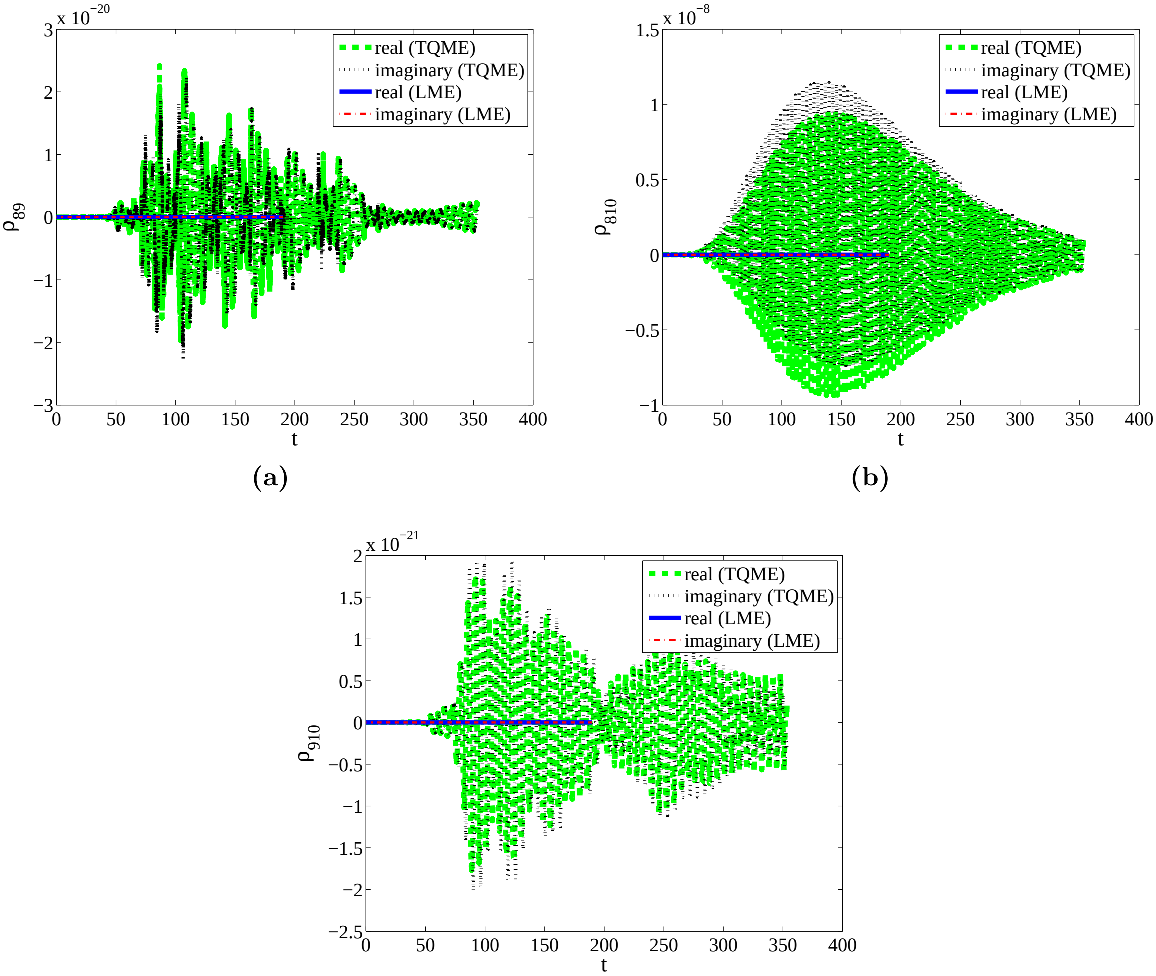


(a) **(b)**

(c) **(d)**

(e) **(f)**

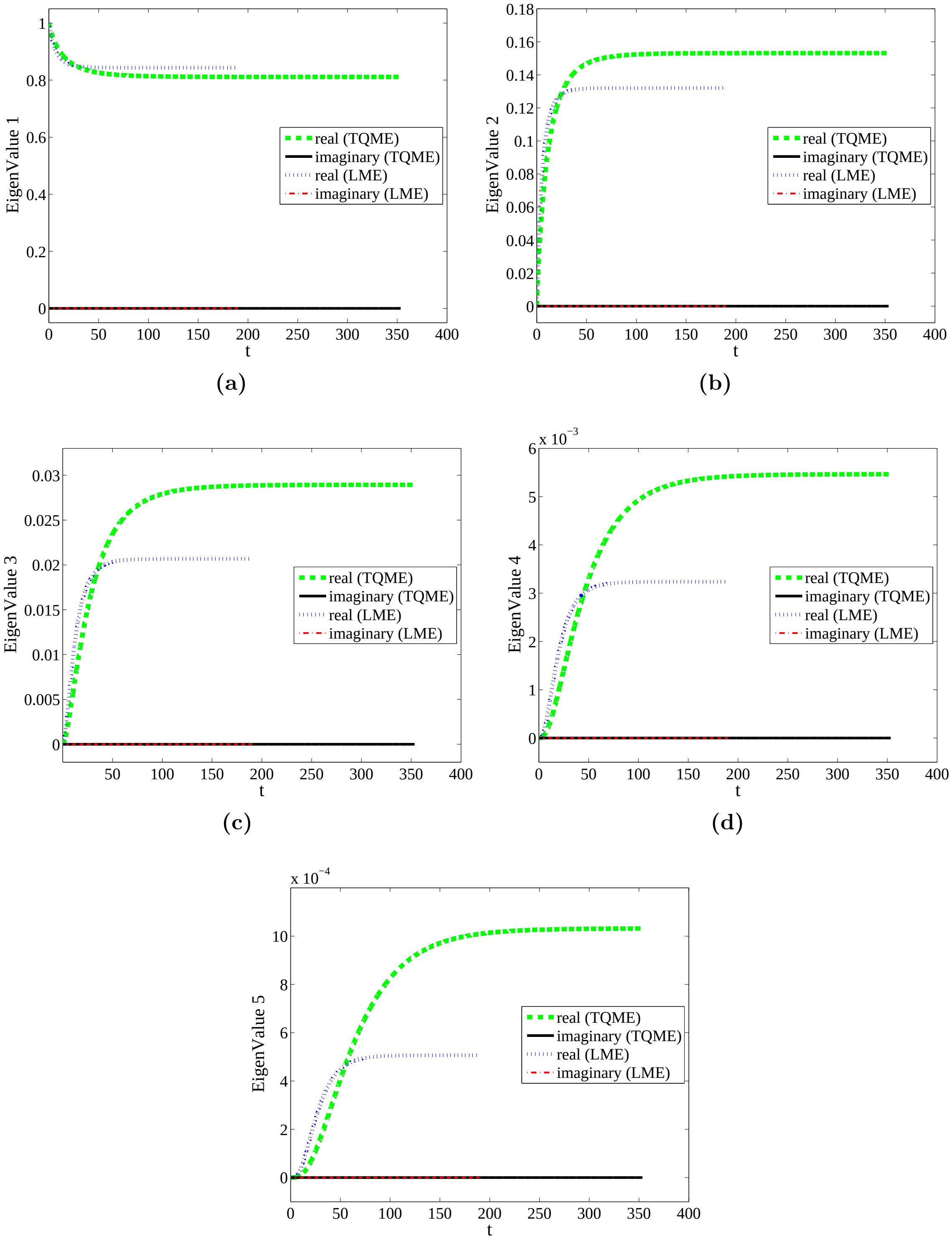
Figure 10.2.1.15: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{68}, ρ_{69}, ρ_{610}, ρ_{78}, ρ_{79}, ρ_{710}.



(a) **(b)**

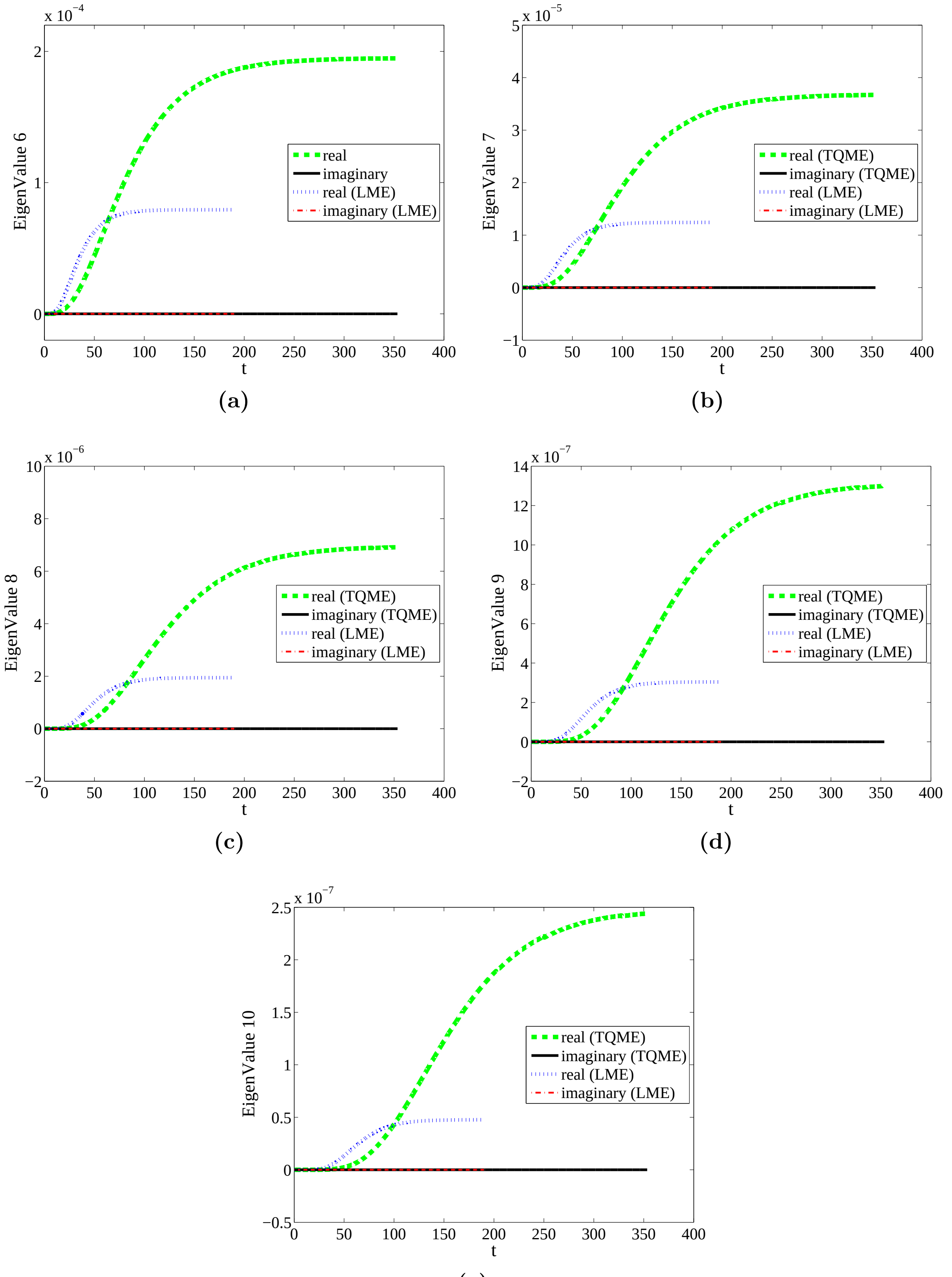
(c)

Figure 10.2.1.16: Same as 10.2.1.7 but for the non-diagonal density matrix elements, ρ_{89}, ρ_{810}, ρ_{910}.



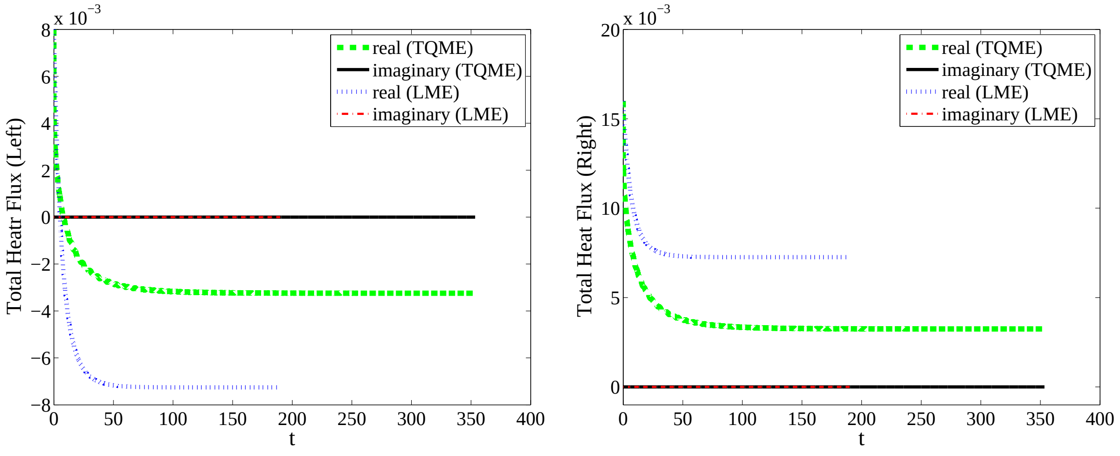
(a) (b) (c) (d) (e)

Figure 10.2.1.17: Same as 10.2.1.7 but for the first five eigenvalues of the density matrix.

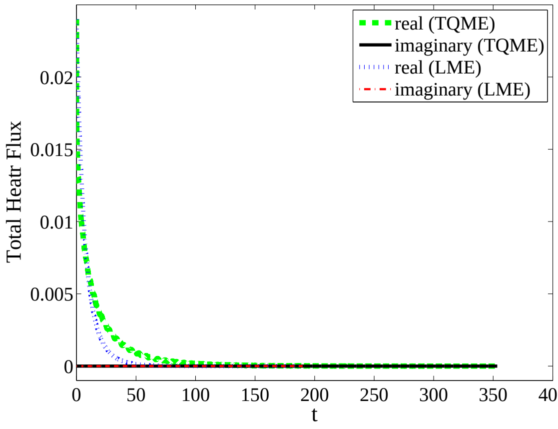


(a) **(b)** **(c)** **(d)** **(e)**

Figure 10.2.1.18: Same as 10.2.1.7 but for the last five eigenvalues of the density matrix.



(a) **(b)**



(c)

Figure 10.2.1.19: Same as 10.2.1.7 but for the heat flux of the left (10.2.1.4a), right (10.2.1.4b) heat baths and the total one (10.2.1.4c).

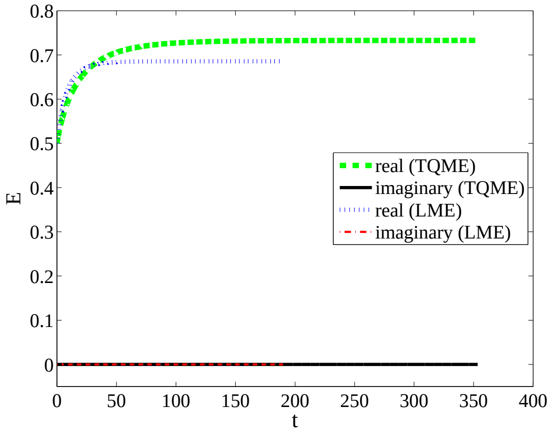
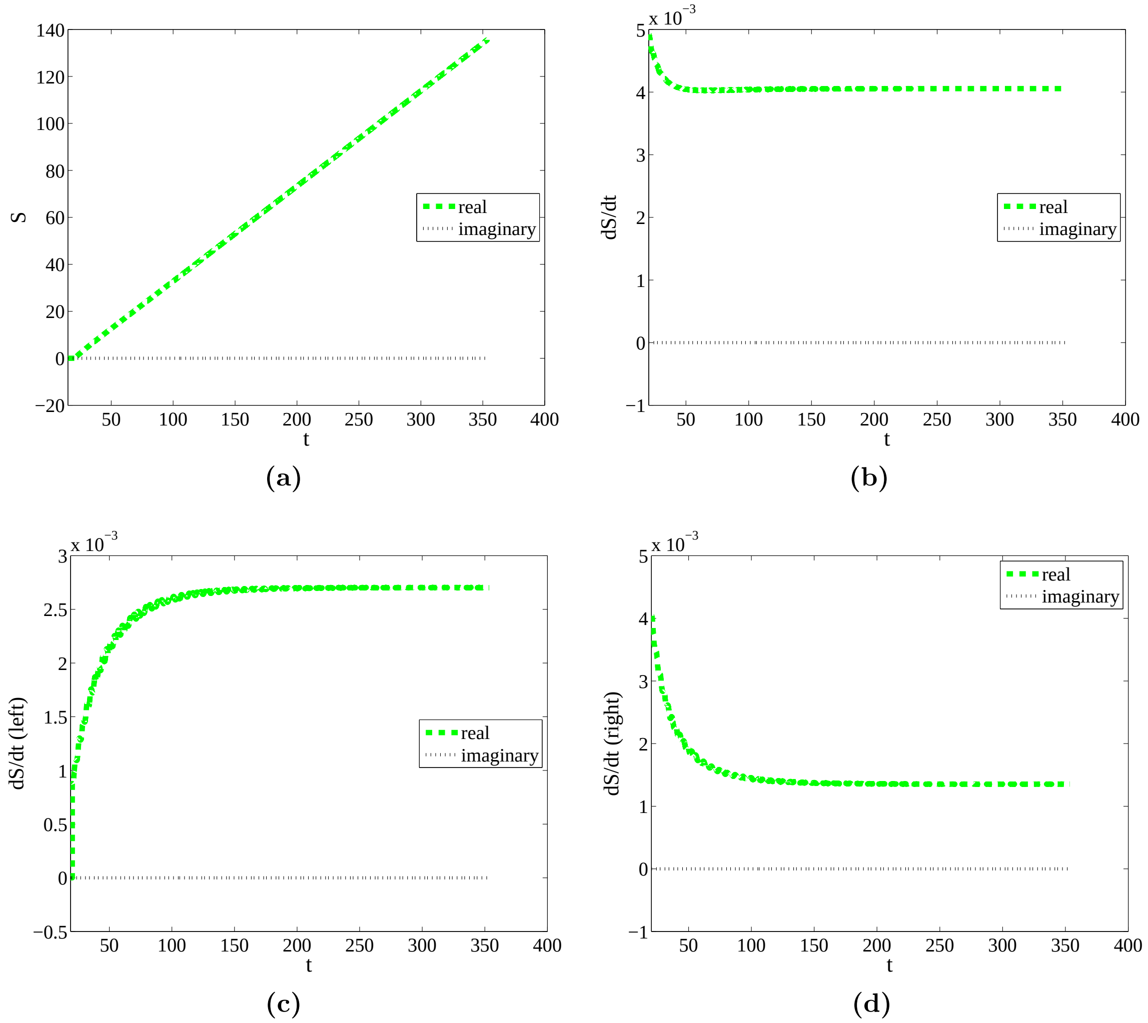


Figure 10.2.1.20: Same as 10.2.1.7 but for the energy E of the system.



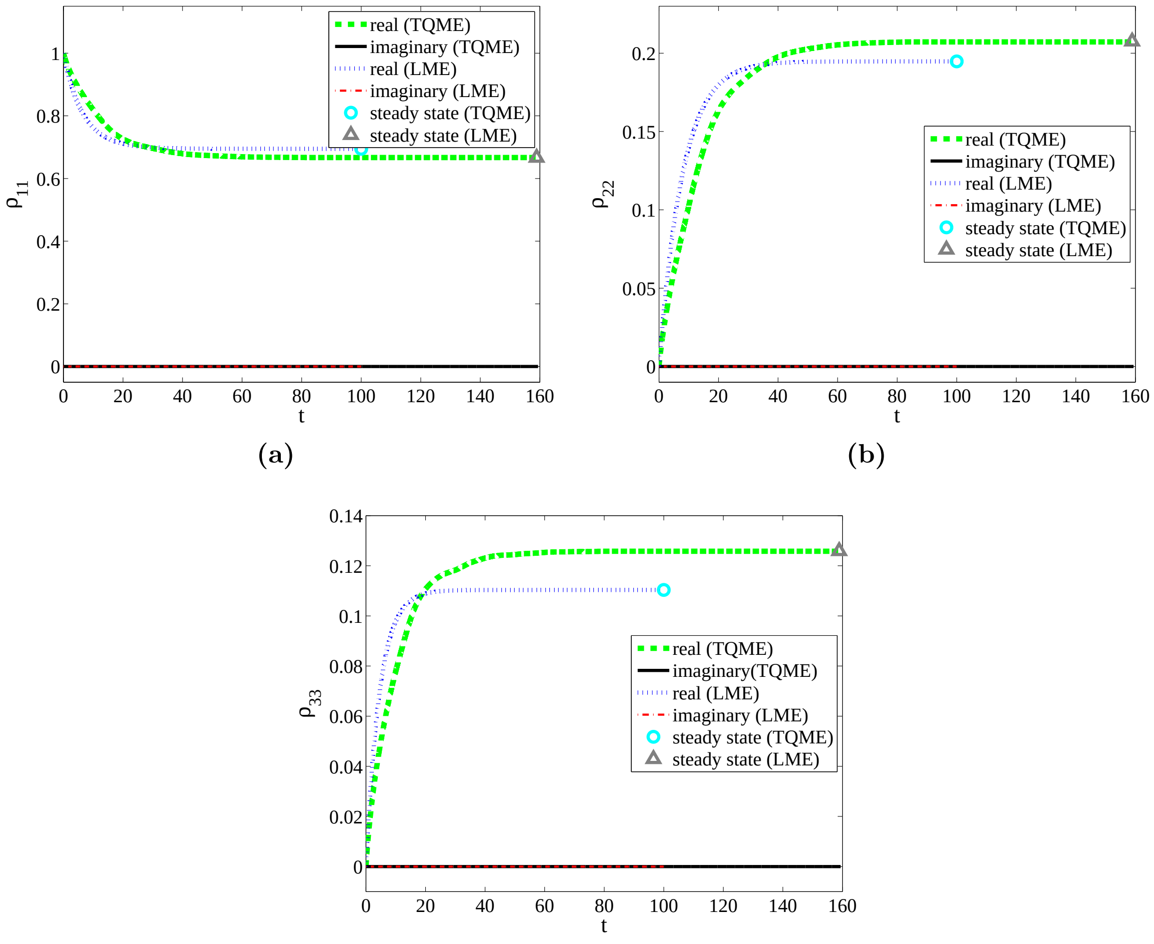
(a) (b) (c) (d)

Figure 10.2.1.21: Time evolution of the real and imaginary part of the entropy S of the system and $\frac{dS}{dt}$, $\frac{dS}{dt}$ (left), $\frac{dS}{dt}$ (right), using the Thermodynamic Quantum Master Equation (TQME) (real (green), imaginary (black)) for the case of the Harmonic Oscillator (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

10.2.2 Direct Steady-State Solution

In this section, we present the results obtained by an independent, non-linear matrix algebra solver that we implemented for computing the steady-state solution of the density matrix. These steady-state solutions are compared with the corresponding values taken from the dynamic relaxation of numerical integration for all the studied occasions.

Three-Level System (Qutrit)



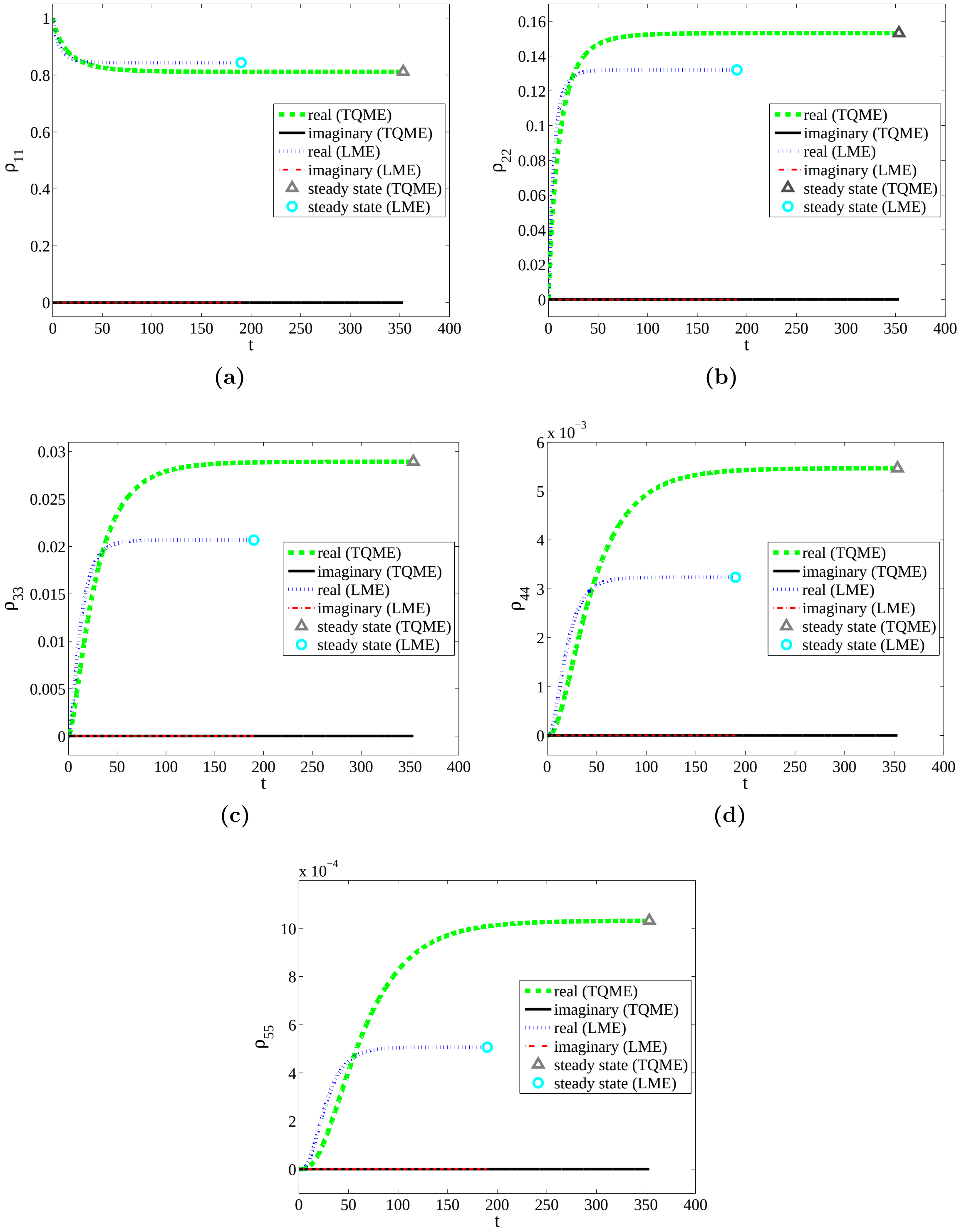
(a)

(b)

(c)

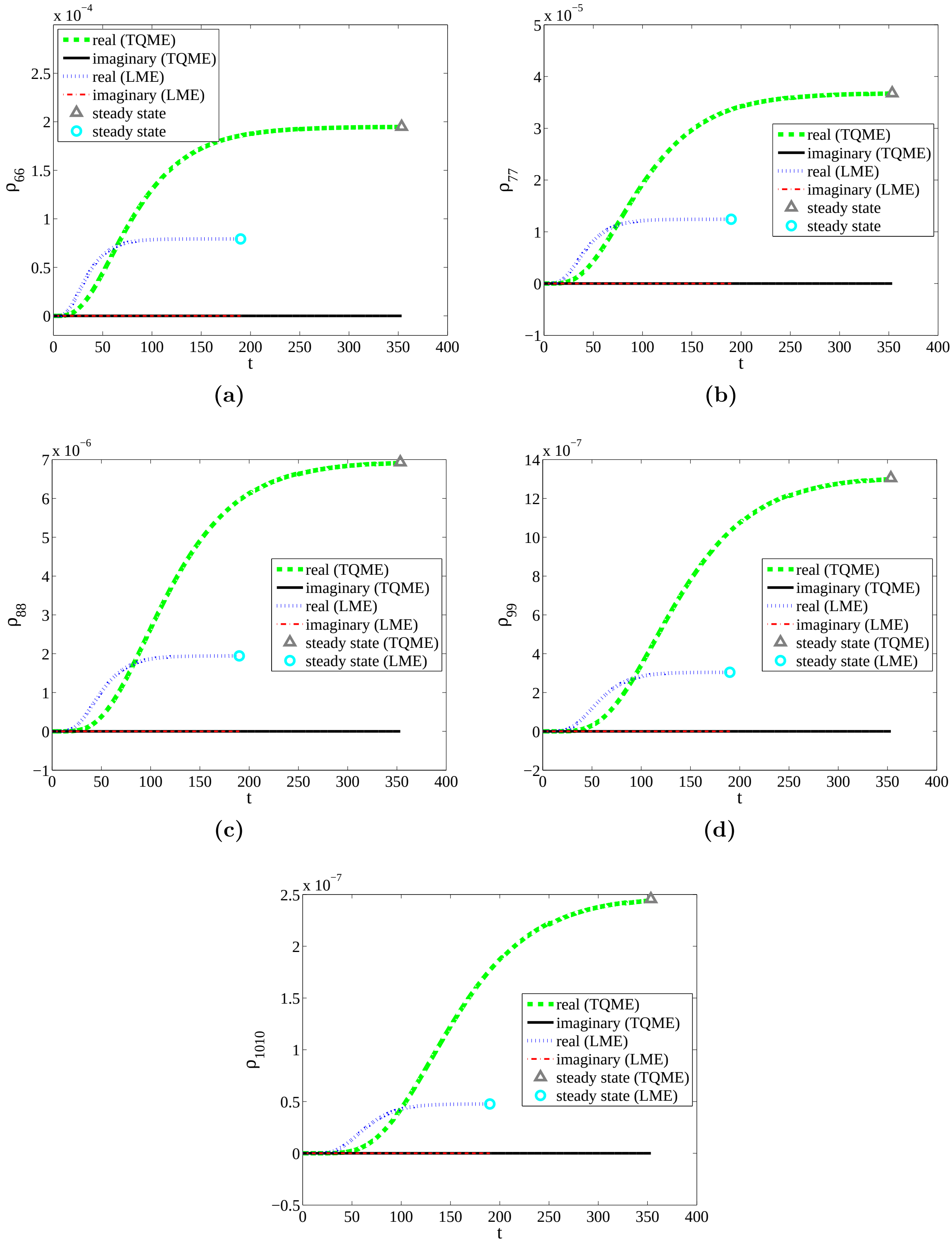
Figure 10.2.2.1: Comparison of the steady-state solution of the diagonal density matrix elements, $\rho_{11}, \rho_{22}, \rho_{33}$, between the time integration and the direct calculation of the steady-state values, using the Lindblad Master Equation (LME) (time integration: real (green), imaginary (black), steady-state solution: real (grey triangular)) and the Thermodynamic Quantum Master Equation (TQME) (time integration: real (blue), imaginary (red), steady-state solution: real (light blue circle)), in the case of the Three-Level system (Qutrit), with $T_l = 0.4$, $T_r = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

Harmonic Oscillator (10 states)



(a) **(b)** **(c)** **(d)** **(e)**

Figure 10.2.2.2: Comparison of the steady-state solution of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, ρ_{44}, ρ_{55}, between the time integration and the direct calculation of the steady-state values, using the Lindblad Master Equation (LME) (time integration: real (green), imaginary (black), steady-state solution: real (grey triangular)) and the Thermodynamic Quantum Master Equation (TQME) (time integration: real (blue), imaginary (red), steady-state solution: real (light blue circle)), in the case of the Harmonic Oscillator (10 states), with $T_l = 0.4$, $T_r = 0.8$ and $\gamma_l = \gamma_r = 0.01$.



(a) (b) (c) (d) (e)

Figure 10.2.2.3: Same as 10.2.2.2 but for ρ_{66}, ρ_{77}, ρ_{88}, ρ_{99}, ρ_{1010}.

10.2.3 Effective Temperatures

Here, we present the effective, steady-state temperature using Eq. 7.3.1 and the steady-state values of the diagonal elements of the density matrix, acquired from the direct steady-state solution in the previous section. The following results refer to both quantum systems, the three-level and the harmonic oscillator, using the Lindblad-type and the Thermodynamic Quantum Master Equation.

	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$
LME	0.6949	0.1947	0.1104
TQME	0.6665	0.2076	0.1259

Table 10.2.3.1: Steady-state solutions for the diagonal density matrix elements using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Three-Level system (Qutrit), with $T_l = 0.4$, $T_r = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

	T_{12}^{eff}	T_{23}^{eff}	T_{13}^{eff}
LME	0.5503	0.5280	0.5434
TQME	0.6000	0.6000	0.6000

Table 10.2.3.2: Effective steady-state temperatures using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Three-Level system (Qutrit), with $T_l = 0.4$, $T_r = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$	$\rho_{44,ss}$	$\rho_{55,ss}$
LME	0.8434	0.1320	0.0207	3.236E-03	5.066E-04
TQME	0.8111	0.1532	0.0289	0.0055	0.0010

Table 10.2.3.3: Steady-state solutions for the first five diagonal density matrix elements using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Harmonic Oscillator system (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

	$\rho_{66,ss}$	$\rho_{77,ss}$	$\rho_{88,ss}$	$\rho_{99,ss}$	$\rho_{1010,ss}$
LME	7.9E-05	1.2E-05	1.9E-06	3.0E-07	4.8E-08
TQME	0.0002	3.676E-05	6.9E-06	1.3E-06	2.5E-07

Table 10.2.3.4: Same as Table 10.2.3.3 for the last five diagonal density matrix elements.

	T_{ij}^{eff}, for $j > i,\ i, j = 1, \ldots, 10$
LME	0.5393
TQME	0.6000

Table 10.2.3.5: Effective steady-state temperatures using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Harmonic Oscillator system (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.01$.

10.2.4 Parametric Analysis

In this section, we present steady-state results for the density matrix and the effective temperatures for a variety of temperature pairs acquired from the direct steady-state solver. These results refer to both quantum systems, the three-level and the harmonic oscillator, using the Lindblad-type and the Thermodynamic Quantum Master Equation.

$T_{e,l}$	$T_{e,r}$	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$
0.1	0.8	0.9916	0.0079	0.0004
0.2	0.8	0.8742	0.0977	0.0281
0.3	0.8	0.7611	0.1619	0.0770
0.4	0.8	0.6950	0.1947	0.1103
0.5	0.8	0.6540	0.2142	0.1318
0.6	0.8	0.6256	0.2273	0.1470
0.7	0.8	0.6042	0.2371	0.1587
0.8	0.8	0.5871	0.2447	0.1682
0.9	0.8	0.5726	0.2511	0.1763
1	0.8	0.5605	0.2563	0.1832

Table 10.2.4.1: Steady-state solutions for the diagonal density matrix elements, referring to the Three-Level system (Qutrit), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.01$.

$T_{e,l}$	$T_{e,r}$	T_{12}^{eff}	T_{23}^{eff}	T_{13}^{eff}
0.1	0.8	0.14	0.10	0.13
0.2	0.8	0.32	0.24	0.29
0.3	0.8	0.45	0.40	0.44
0.4	0.8	0.55	0.53	0.54
0.5	0.8	0.63	0.62	0.62
0.6	0.8	0.69	0.69	0.69
0.7	0.8	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85
1	0.8	0.89	0.89	0.89

Table 10.2.4.2: Effective steady-state temperatures, referring to the Three-Level system (Qutrit), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, $T_{e,l}$ and $T_{e,r}$, and $\gamma_l = \gamma_r = 0.01$.

T_l	T_r	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$
0.1	0.8	0.7579	0.1599	0.0821
0.2	0.8	0.7236	0.1784	0.0979
0.3	0.8	0.6933	0.1942	0.1125
0.4	0.8	0.6665	0.2076	0.1259
0.5	0.8	0.6429	0.2190	0.1380
0.6	0.8	0.6221	0.2289	0.1491
0.7	0.8	0.6036	0.2373	0.1591
0.8	0.8	0.5871	0.2447	0.1682
0.9	0.8	0.5723	0.2512	0.176
1	0.8	0.5591	0.2568	0.1840

Table 10.2.4.3: Steady-state solutions for the diagonal density matrix elements, referring to the Three-Level system (Qutrit), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.01$.

T_l	T_r	T_{12}^{eff}	T_{23}^{eff}	T_{13}^{eff}
0.1	0.8	0.45	0.45	0.45
0.2	0.8	0.50	0.50	0.50
0.3	0.8	0.55	0.55	0.55
0.4	0.8	0.60	0.60	0.60
0.5	0.8	0.65	0.65	0.65
0.6	0.8	0.70	0.70	0.70
0.7	0.8	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85
1	0.8	0.90	0.90	0.90

Table 10.2.4.4: Effective steady-state temperatures, referring to the Three-Level system (Qutrit), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, $T_{E,l}$ and $T_{e,r}$, and $\gamma_l = \gamma_r = 0.01$.

T_l	T_r	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$	$\rho_{44,ss}$	$\rho_{55,ss}$
0.1	0.8	0.9996	4.0791E-04	1.7E-07	6.8E-11	2.8E-14
0.2	0.8	0.9692	0.0298	0.000919012	2.82992E-05	8.7E-07
0.3	0.8	0.9018	0.0886	0.008696108	8.53947E-04	8.3857E-05
0.4	0.8	0.8434	0.1320	0.02067123	0.0032	5.0661E-04
0.5	0.8	0.7996	0.1602	0.032113877	0.0064	0.0013
0.6	0.8	0.7654	0.1795	0.042110026	0.0099	0.0023
0.7	0.8	0.7374	0.1936	0.050833087	0.0133	0.0035
0.8	0.8	0.7135	0.2044	0.058567457	0.0168	0.0048
0.9	0.8	0.69225	0.2131	0.065549415	0.0202	0.0062
1	0.8	0.6734	0.2199	0.07184711	0.0235	0.0077

Table 10.2.4.5: Steady-state solutions for the first five diagonal density matrix elements, referring to the Harmonic Oscillator system (10 states), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.01$.

T_l	T_r	$\rho_{66,ss}$	$\rho_{77,ss}$	$\rho_{88,ss}$	$\rho_{99,ss}$	$\rho_{1010,ss}$
0.1	0.8	1.1E-17	4.6E-21	1.9E-24	6.4E-28	3.1E-31
0.2	0.8	2.7E-08	8.3E-10	2.5E-11	7.8E-13	2.4E-14
0.3	0.8	8.2346E-06	8.1E-07	7.9E-08	7.8E-09	7.6E-10
0.4	0.8	7.931E-05	1.2415E-05	1.9E-06	3.0E-07	4.8E-08
0.5	0.8	2.5848E-04	5.1802E-05	1.0381E-05	2.1E-06	4.2E-07
0.6	0.8	5.4334E-04	1.2743E-04	2.9891E-05	7.0E-06	1.6E-06
0.7	0.8	9.2E-04	2.4154E-04	6.3418E-05	1.6650E-05	4.4E-06
0.8	0.8	0.0014	3.9462E-04	1.1306E-04	3.2393E-05	9.3E-06
0.9	0.8	0.0019	5.8700E-04	1.8057E-04	5.5550E-05	1.7088E-05
1	0.8	0.0025	8.1792E-04	2.6717E-04	8.7270E-05	2.8507E-05

Table 10.2.4.6: Same as Table 10.2.4.5 but for the last five diagonal density matrix elements.

$T_{e,l}$	$T_{e,r}$	T_{12}^{eff}	T_{23}^{eff}	T_{34}^{eff}	T_{45}^{eff}	T_{56}^{eff}
0.1	0.8	0.13	0.13	0.13	0.13	0.13
0.2	0.8	0.29	0.29	0.29	0.29	0.29
0.3	0.8	0.43	0.43	0.43	0.43	0.43
0.4	0.8	0.54	0.54	0.54	0.54	0.54
0.5	0.8	0.62	0.62	0.62	0.62	0.62
0.6	0.8	0.69	0.69	0.69	0.69	0.69
0.7	0.8	0.75	0.75	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85	0.85	0.85
1	0.8	0.89	0.89	0.89	0.89	0.89

Table 10.2.4.7: Effective steady-state temperatures for the first five transitions, referring to the Harmonic Oscillator system (10 states), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.01$.

$T_{e,l}$	$T_{e,r}$	T_{67}^{eff}	T_{78}^{eff}	T_{89}^{eff}	T_{910}^{eff}
0.1	0.8	0.13	0.13	0.13	0.13
0.2	0.8	0.29	0.29	0.29	0.29
0.3	0.8	0.43	0.43	0.43	0.43
0.4	0.8	0.54	0.54	0.54	0.54
0.5	0.8	0.62	0.62	0.62	0.62
0.6	0.8	0.69	0.69	0.69	0.69
0.7	0.8	0.77	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85	0.85
1	0.8	0.89	0.89	0.89	0.89

Table 10.2.4.8: Same as 10.2.4.7 for the last four transitions.

$T_{e,l}$	$T_{e,r}$	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$	$\rho_{44,ss}$	$\rho_{55,ss}$
0.1	0.8	0.8916	0.0966	0.0105	0.0011	1.2297E-04
0.2	0.8	0.8647	0.1170	0.0158	0.0021	2.9006E-04
0.3	0.8	0.8377	0.1360	0.0221	0.0036	5.8153E-04
0.4	0.8	0.8111	0.1532	0.0289	0.0055	0.0010
0.5	0.8	0.7857	0.1684	0.0361	0.0077	0.0016
0.6	0.8	0.7603	0.1822	0.0437	0.0105	0.0025
0.7	0.8	0.7364	0.1941	0.0511	0.0135	0.0035
0.8	0.8	0.7135	0.2044	0.0586	0.0168	0.0048
0.9	0.8	0.6916	0.2133	0.0658	0.0203	0.0062
1	0.8	0.6708	0.2208	0.0727	0.0239	0.0079

Table 10.2.4.9: Steady-state solutions for the first five diagonal density matrix elements, referring to the Harmonic Oscillator system (10 states), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, $T_{e,l}$ and $T_{e,r}$, and $\gamma_l = \gamma_r = 0.01$.

$T_{e,l}$	$T_{e,r}$	$\rho_{66,ss}$	$\rho_{77,ss}$	$\rho_{88,ss}$	$\rho_{99,ss}$	$\rho_{1010,ss}$
0.1	0.8	1.3326E-05	1.4E-06	1.6E-07	1.7E-08	1.8E-09
0.2	0.8	3.9256E-05	5.3E-06	7.2E-07	9.7E-08	1.3E-08
0.3	0.8	9.4394E-05	1.5322E-05	2.5E-06	4.0E-07	6.5E-08
0.4	0.8	1.94859E-04	3.6769E-05	6.9E-06	1.3E-06	2.4E-07
0.5	0.8	3.5366E-04	7.5524E-05	1.6097E-05	3.4E-06	7.3E-07
0.6	0.8	6.0105E-04	1.4404E-04	3.4520E-05	8.3E-06	2.0E-06
0.7	0.8	9.3717E-04	2.4704E-04	6.5118E-05	1.7165E-05	4.52E-06
0.8	0.8	0.0014	3.9462E-04	1.1306E-04	3.2393E-05	9.3E-06
0.9	0.8	0.0019	5.9466E-04	1.8344E-04	5.6546E-05	1.7437E-05
1	0.8	0.0026	8.5370E-04	2.8103E-04	9.2514E-05	3.0455E-05

Table 10.2.4.10: Same as Table 10.2.4.9 but for the last five diagonal density matrix elements.

T_l	T_r	T_{12}^{eff}	T_{23}^{eff}	T_{34}^{eff}	T_{45}^{eff}	T_{56}^{eff}
0.1	0.8	0.45	0.45	0.45	0.45	0.45
0.2	0.8	0.50	0.50	0.50	0.50	0.50
0.3	0.8	0.55	0.55	0.55	0.55	0.55
0.4	0.8	0.60	0.60	0.60	0.60	0.55
0.5	0.8	0.65	0.65	0.65	0.65	0.65
0.6	0.8	0.70	0.70	0.70	0.70	0.70
0.7	0.8	0.75	0.75	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85	0.85	0.85
1	0.8	0.90	0.90	0.90	0.90	0.90

Table 10.2.4.11: Effective steady-state temperatures for the first five transitions, referring to the Harmonic Oscillator system (10 states), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.01$.

T_l	T_r	T_{67}^{eff}	T_{78}^{eff}	T_{89}^{eff}	T_{910}^{eff}
0.1	0.8	0.450000014	0.450000018	0.45000002	0.450000022
0.2	0.8	0.500000002	0.500000002	0.500000002	0.500000002
0.3	0.8	0.549999739	0.54999976	0.549999762	0.549999762
0.4	0.8	0.599653821	0.599305437	0.598831861	0.598663963
0.5	0.8	0.647713735	0.646896873	0.645945614	0.645631154
0.6	0.8	0.7	0.700000001	0.700000001	0.700000001
0.7	0.8	0.749999999	0.749999999	0.75	0.750000001
0.8	0.8	0.799999744	0.799999744	0.799999745	0.799999746
0.9	0.8	0.850000004	0.850000005	0.850000007	0.850000008
1	0.8	0.900000005	0.900000006	0.900000008	0.90000001

Table 10.2.4.12: Same as Table 10.2.4.11 but for the last four transitions.

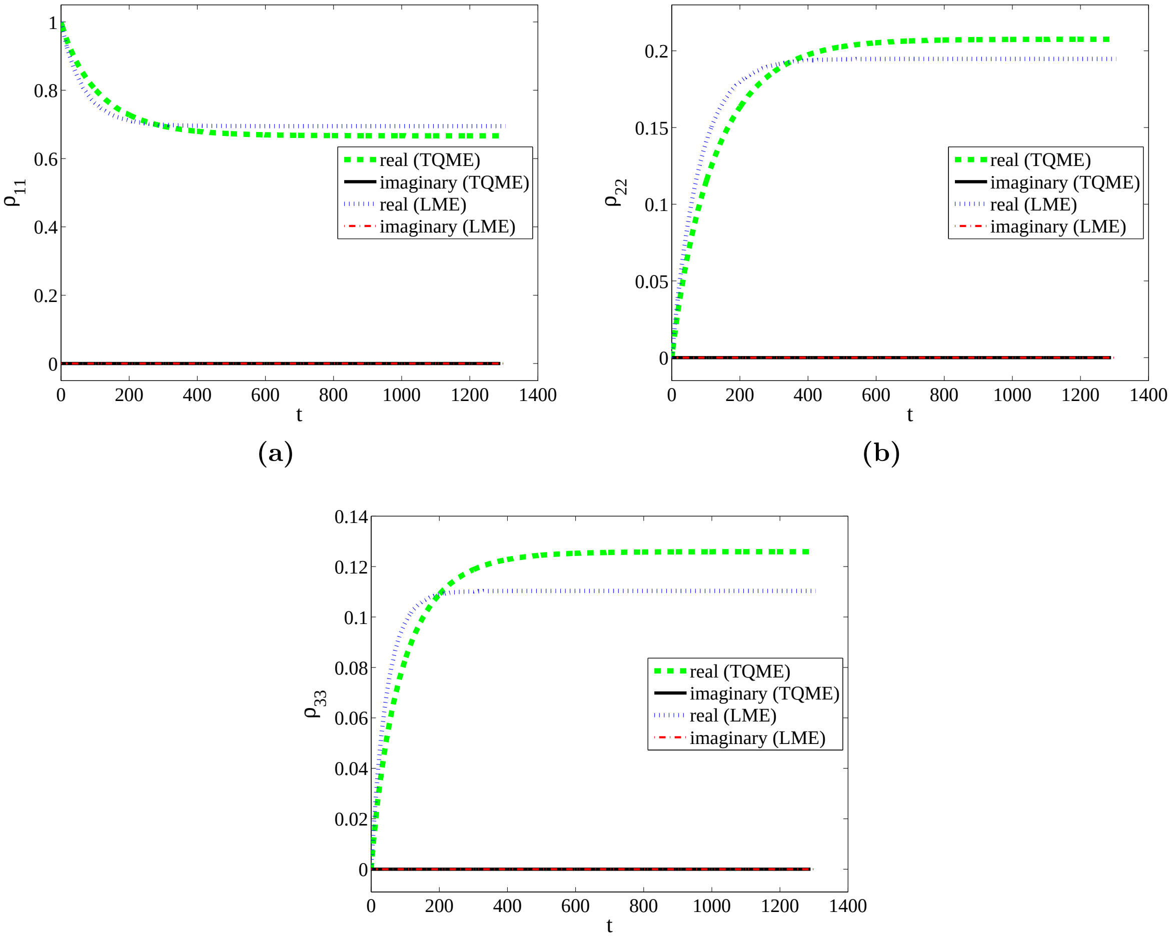
10.3 Quantum Susbsystem coupled to Two Heat Baths - 2^{nd} Set

In this section, results are presented that have been obtained through the time integration and the direct calculation of the steady-state values using the Lindblad Master Equation (LME), Eq. 7.1.2, and the Thermodynamic Quantum Master Equation (TQME), Eq. 7.2.4.1. These results refer to the two cases that we study; the three-level and the harmonic oscillator as quantum subsystems coupled to two heat baths. The inputs where the same mentioned in section 9.2, with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

10.3.1 Time Integration

The integration scheme used in this work is the Adams-Bashforth 4th order ($s = 4$) in Eq. 8.1.4) with the help of single-step Euler's scheme in order to obtain the four starting values. The integration time step that we set was $h = 10^{-2}$.

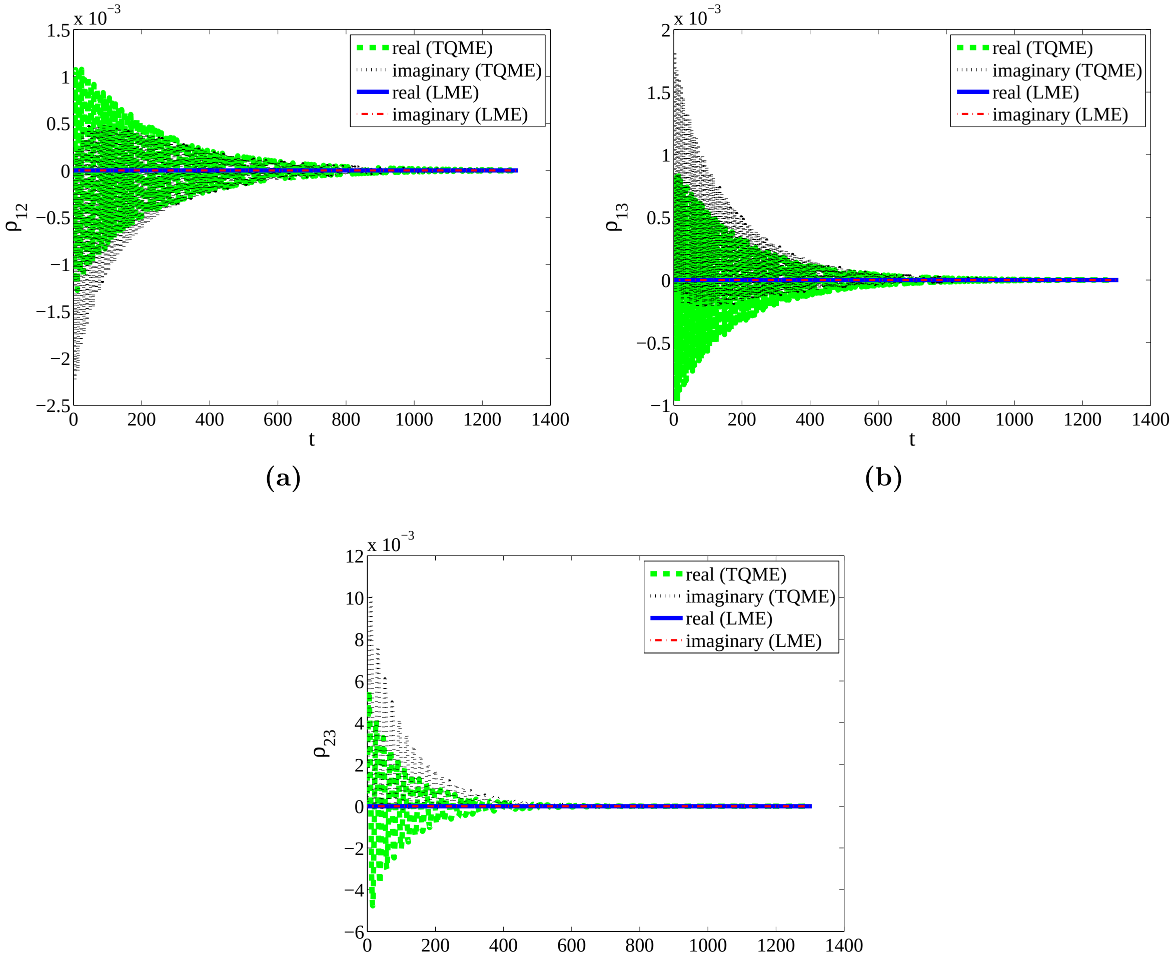
Three-Level System (Qutrit)



(a) **(b)**

(c)

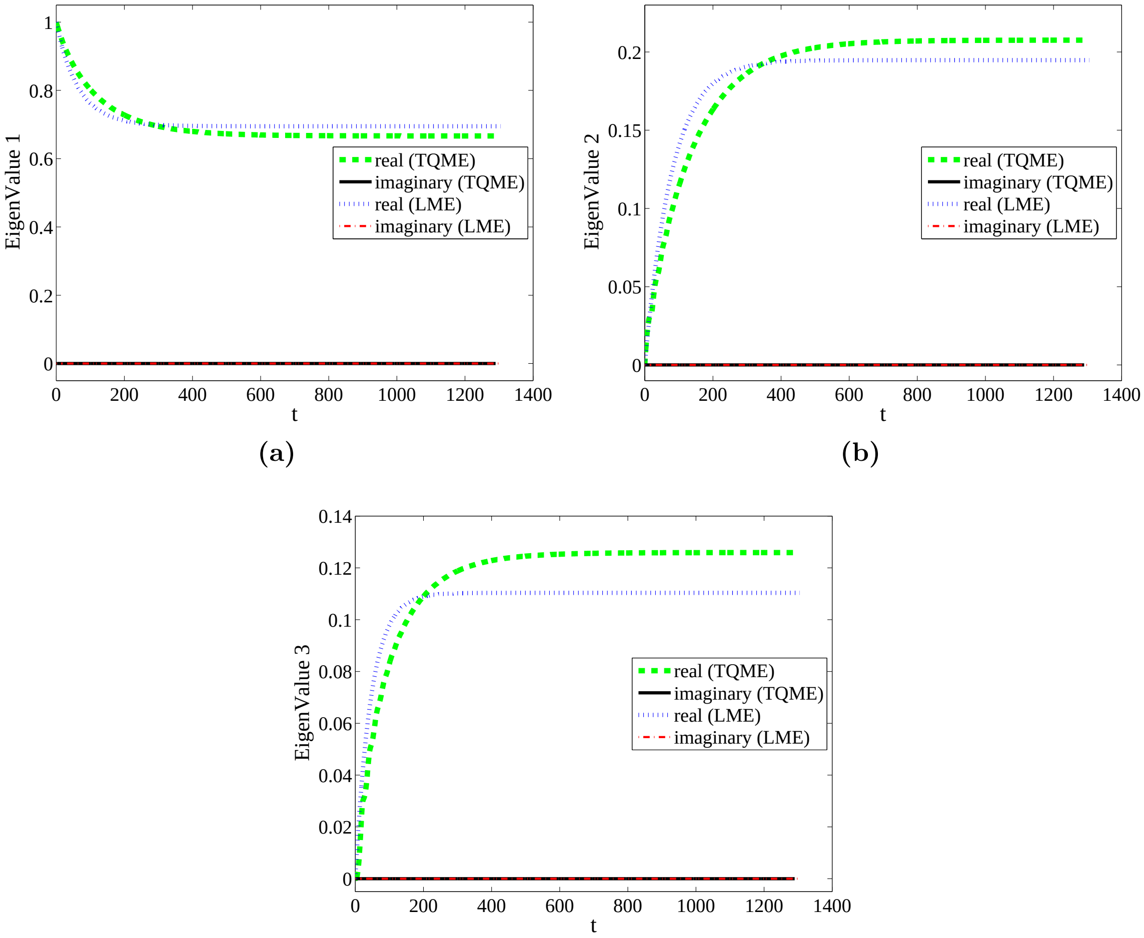
Figure 10.3.1.1: Time evolution of the real and imaginary part of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, using the Lindblad Master Equation (LME) (real (green), imaginary (black)) and the Thermodynamic Quantum Master Equation (TQME) (real (blue), imaginary (red)) for the case of the Three-Level system (Qutrit), with $T_{e,l}$ = 0.4, $T_{e,r}$ = 0.8 and γ_l = γ_r = 0.001.



(a) **(b)**

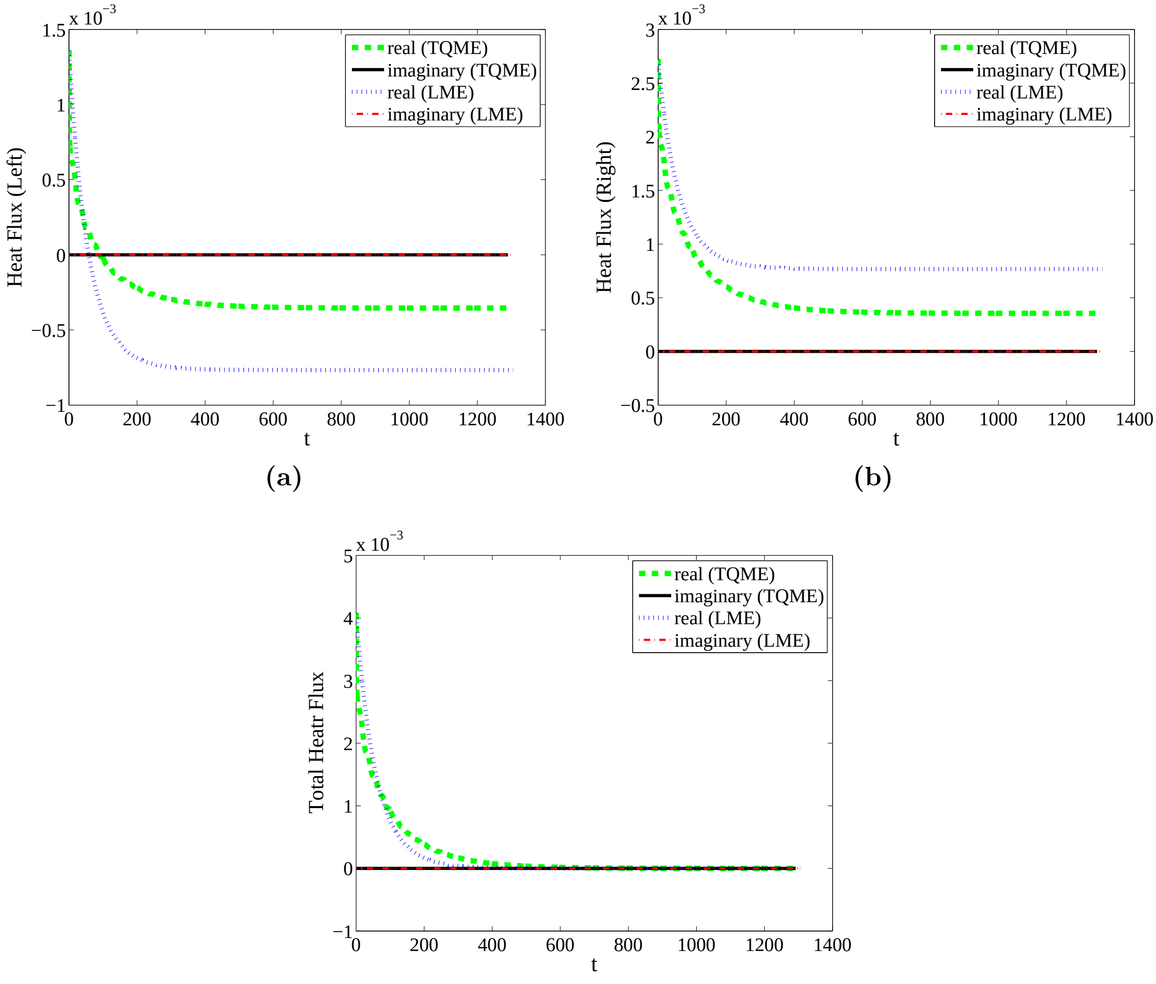
(c)

Figure 10.3.1.2: Same as 10.3.1.1 but for the non-diagonal density matrix elements, ρ_{12}, ρ_{13}, ρ_{23}.



(a) (b) (c)

Figure 10.3.1.3: Same as 10.3.1.1 but for the eigenvalues of the density matrix.



(a)

(b)

(c)

Figure 10.3.1.4: Same as 10.3.1.1 but for the heat flux of the left (10.3.1.4a), right (10.3.1.4b) heat baths and the total one (10.3.1.4c).

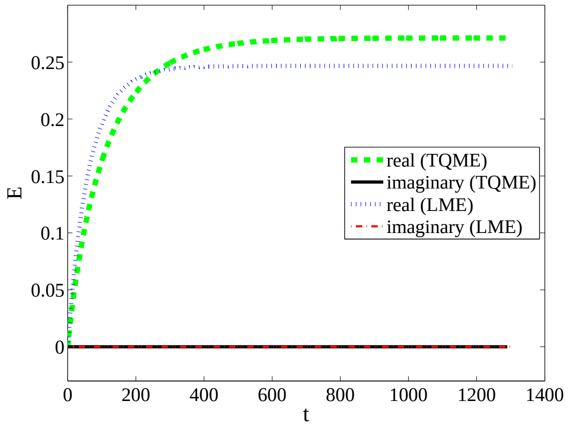
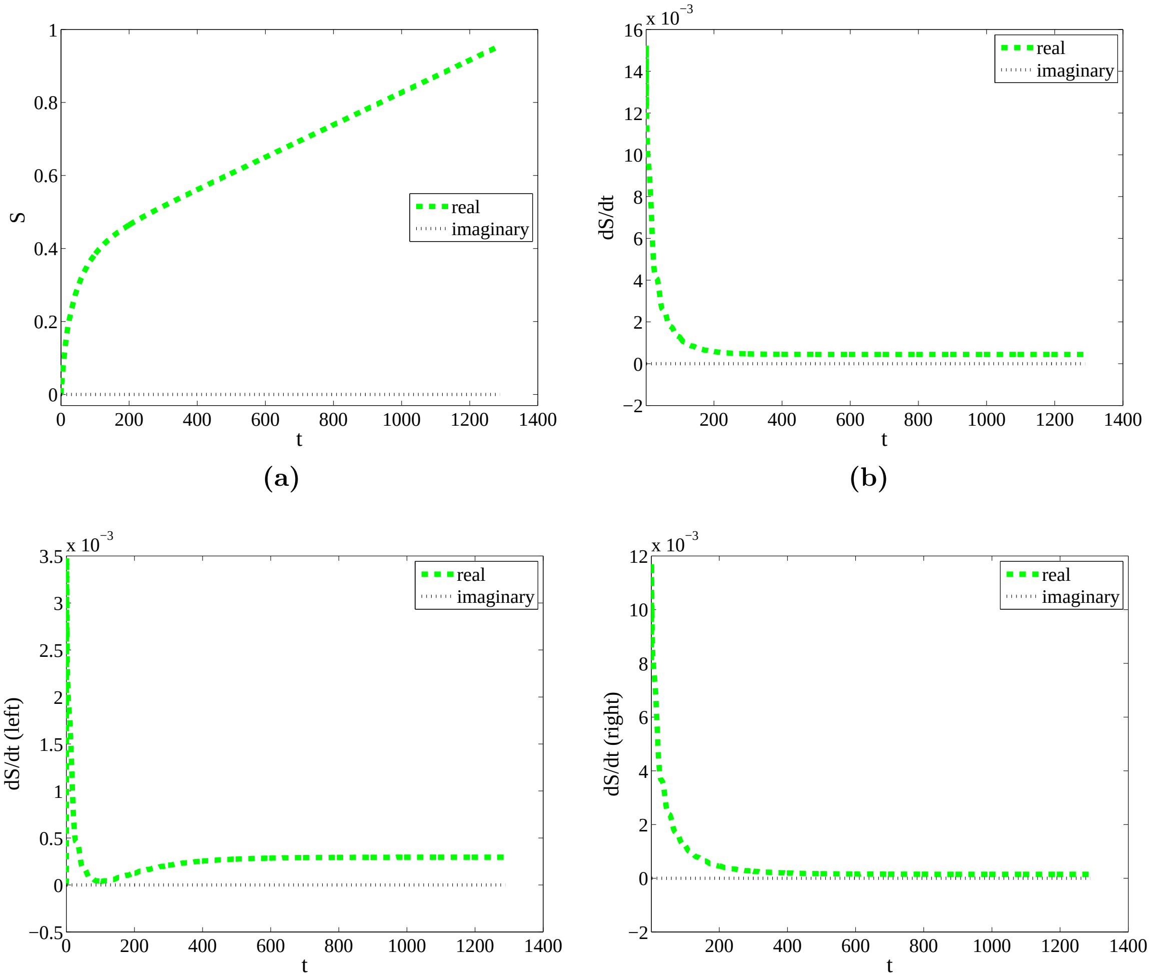


Figure 10.3.1.5: Same as 10.3.1.1 but for the energy E of the system.

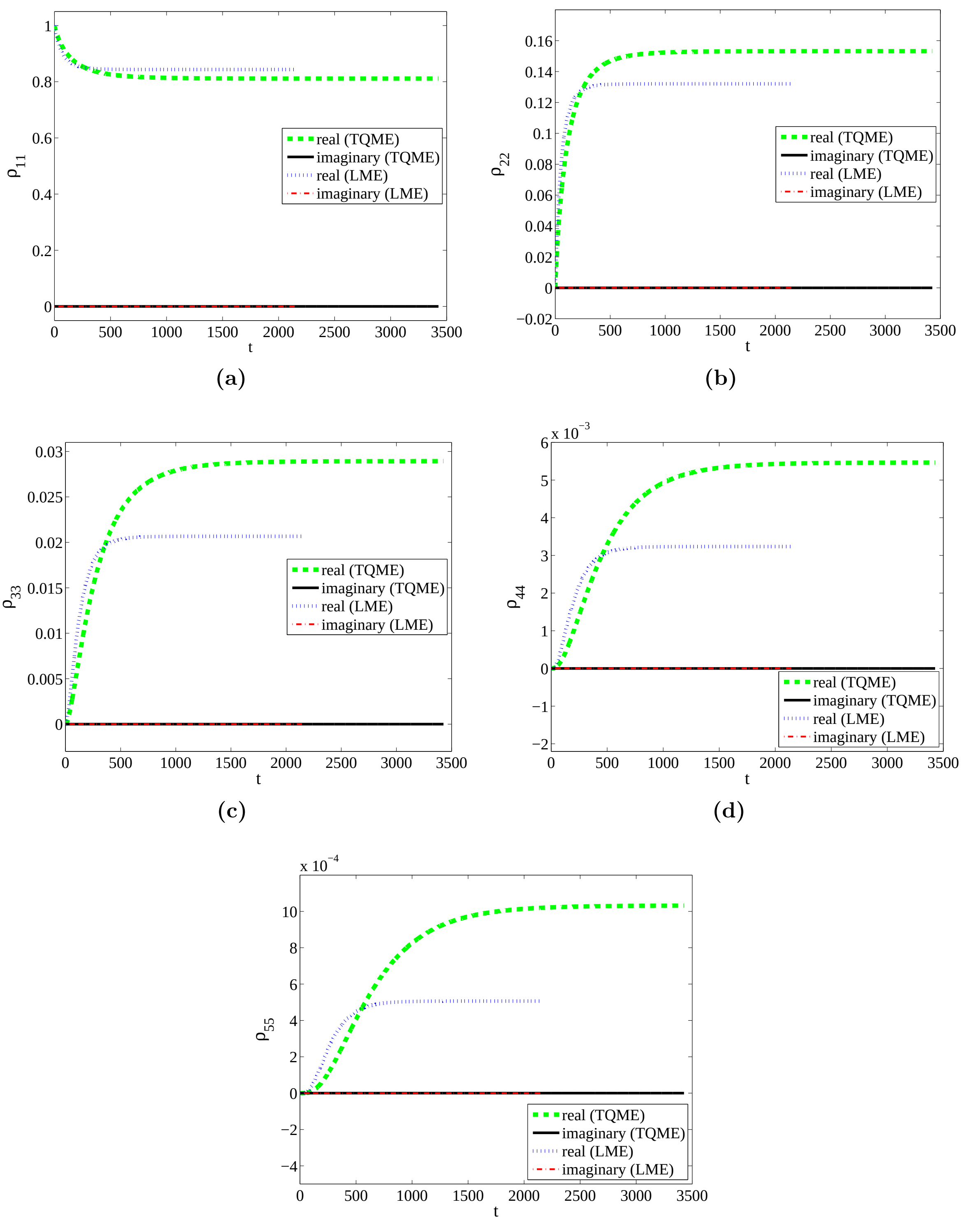


(a) **(b)**

(c) **(d)**

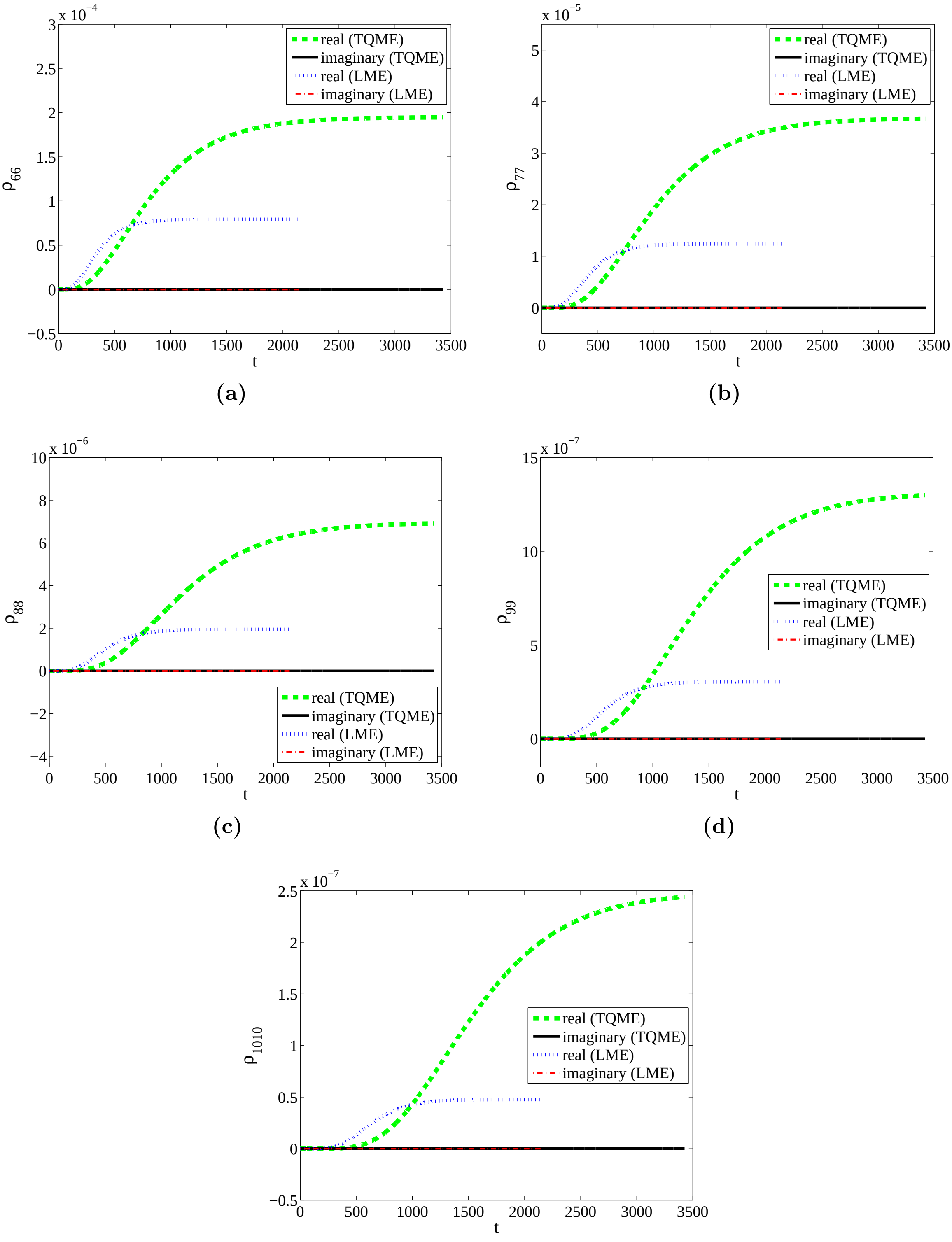
Figure 10.3.1.6: Time evolution of the real and imaginary part of the entropy S of the system and $\frac{dS}{dt}$, $\frac{dS}{dt}$ (left), $\frac{dS}{dt}$ (right), using the Thermodynamic Quantum Master Equation (TQME) (real (green), imaginary (black)) for the case of the Three-Level system (Qutrit), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

Harmonic Oscillator (10 states)



(a) (b) (c) (d) (e)

Figure 10.3.1.7: Time evolution of the real and imaginary part of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, using the Lindblad Master Equation (LME) (real (green), imaginary (black)) and the Thermodynamic Quantum Master Equation (TQME) (real (blue), imaginary (red)) for the case of the Harmonic Oscillator (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

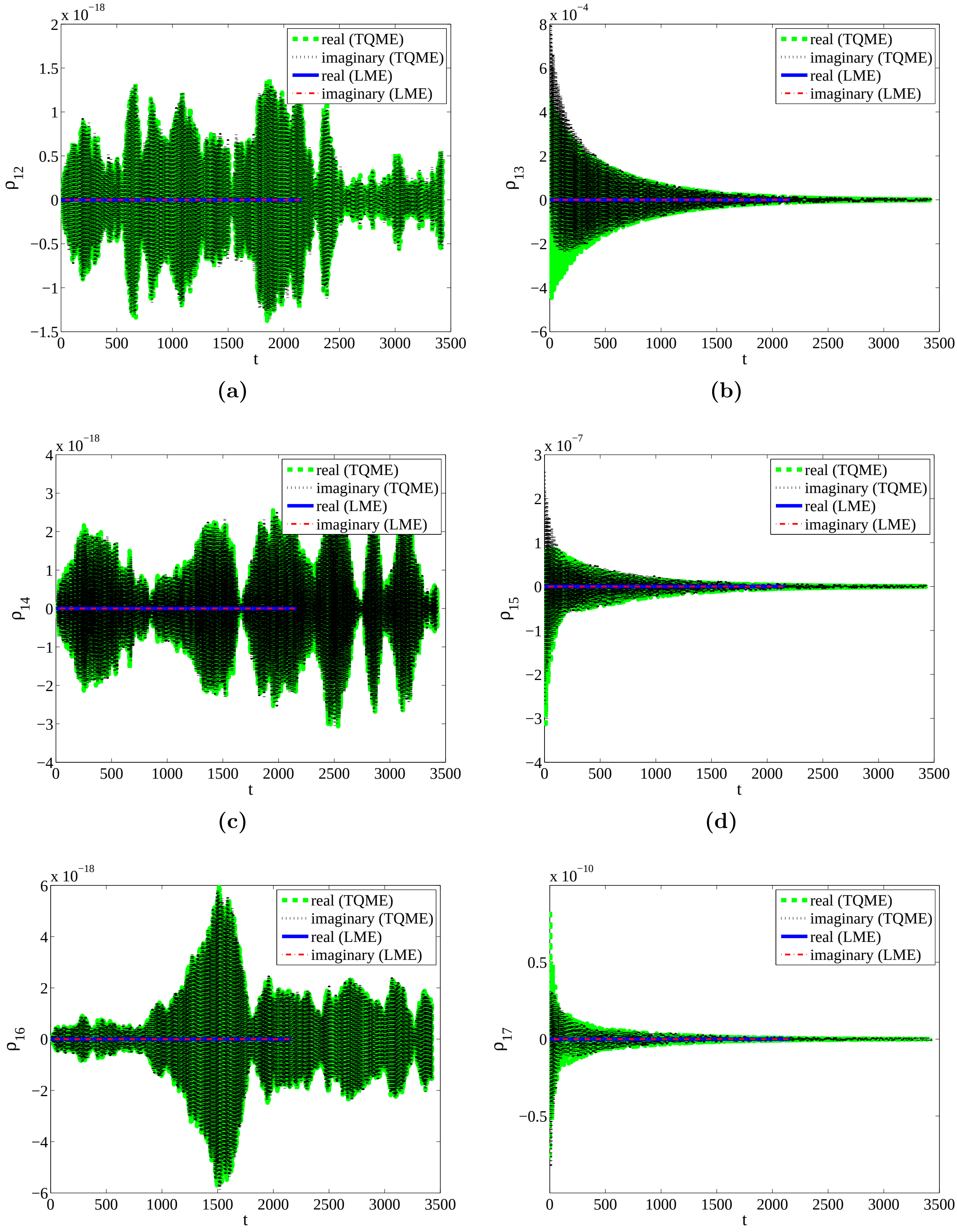


(a) **(b)**

(c) **(d)**

(e)

Figure 10.3.1.8: Same as 10.3.1.7 but for the diagonal density matrix elements, ρ_{66}, ρ_{77}, ρ_{88}, ρ_{99}, ρ_{1010}.

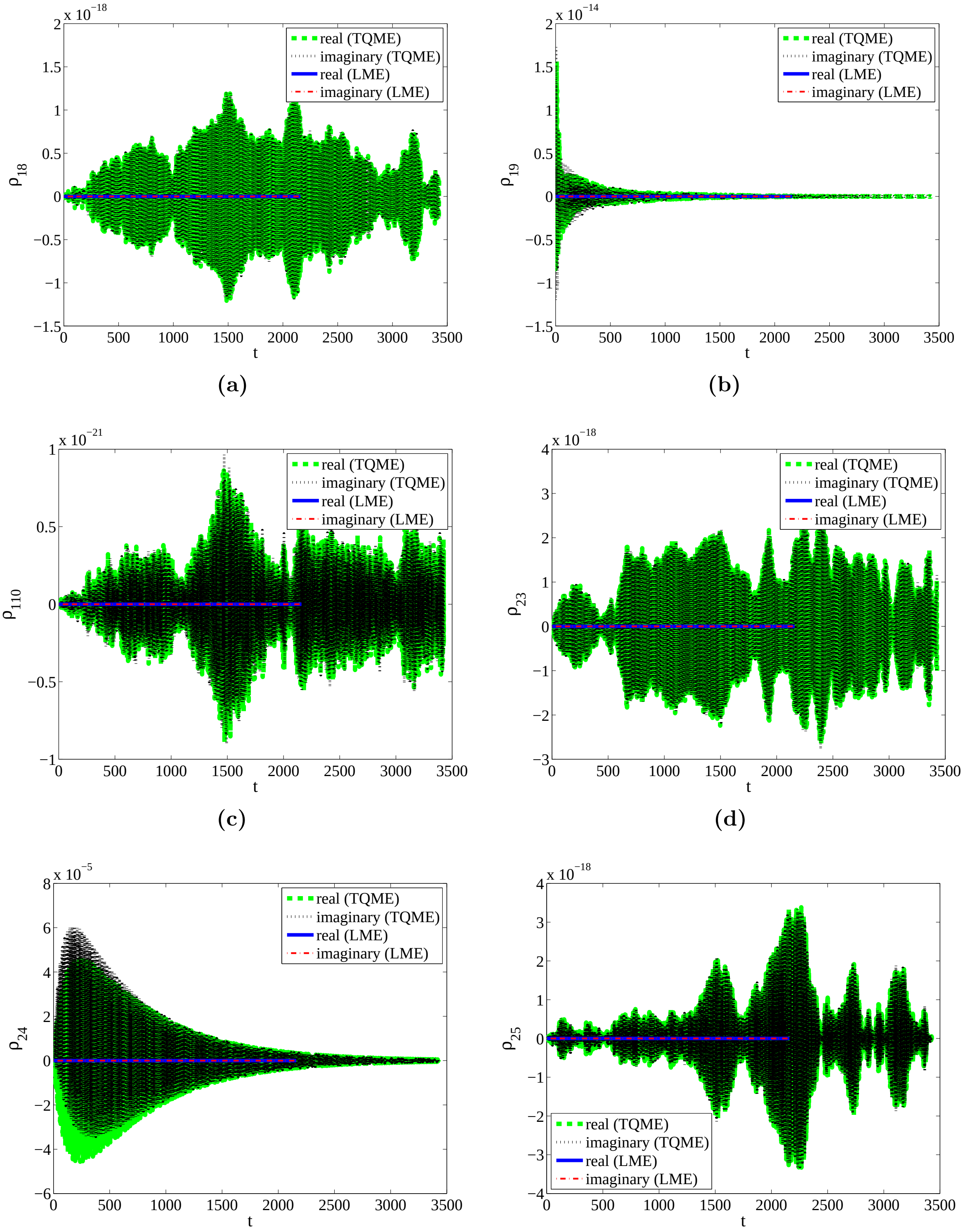


(a) (b)

(c) (d)

(e) (f)

Figure 10.3.1.9: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{12}, ρ_{13}, ρ_{14}, ρ_{15}, ρ_{16}, ρ_{17}.



(a)

(b)

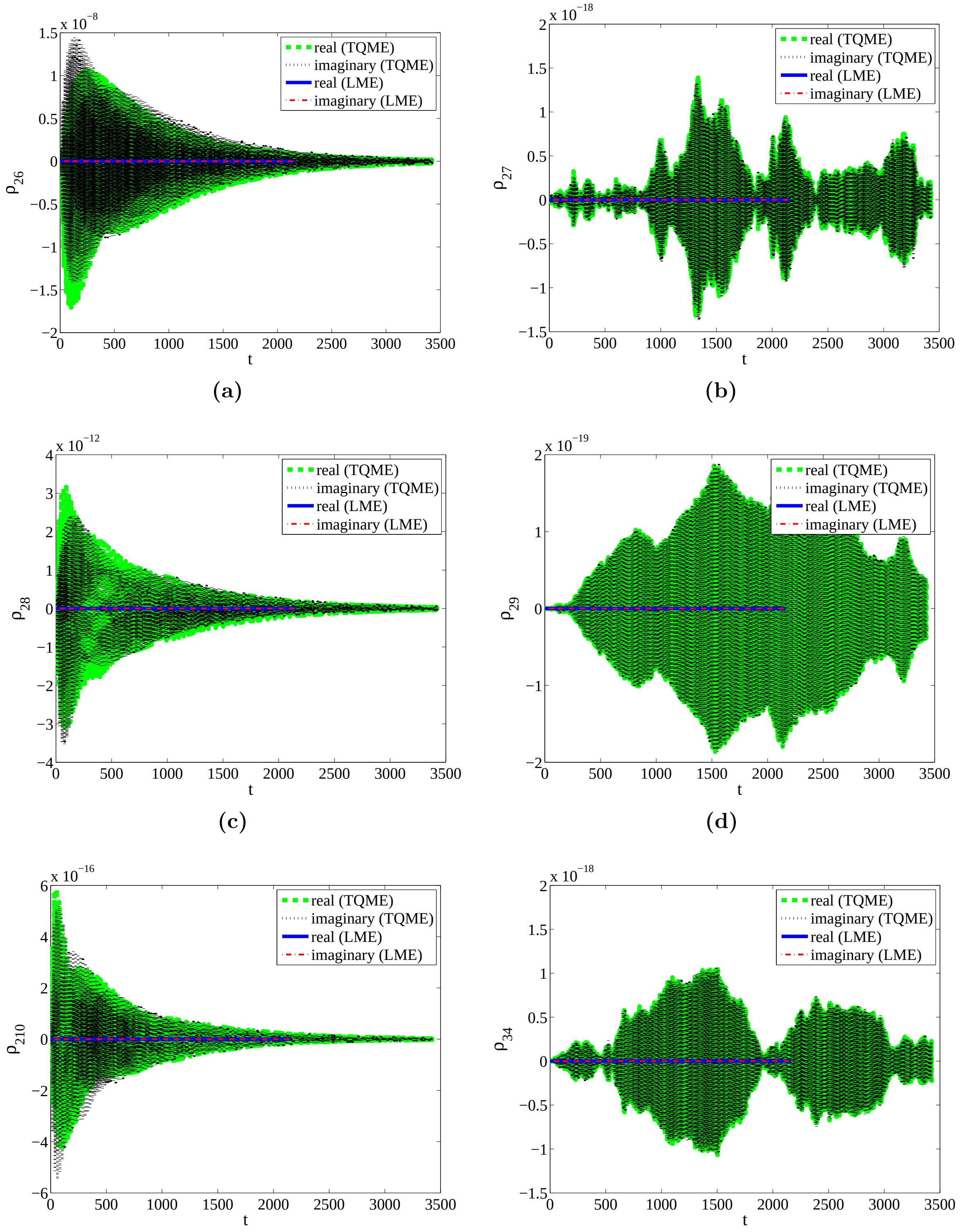
(c)

(d)

(e)

(f)

Figure 10.3.1.10: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{18}, ρ_{19}, ρ_{110}, ρ_{23}, ρ_{24}, ρ_{25}.

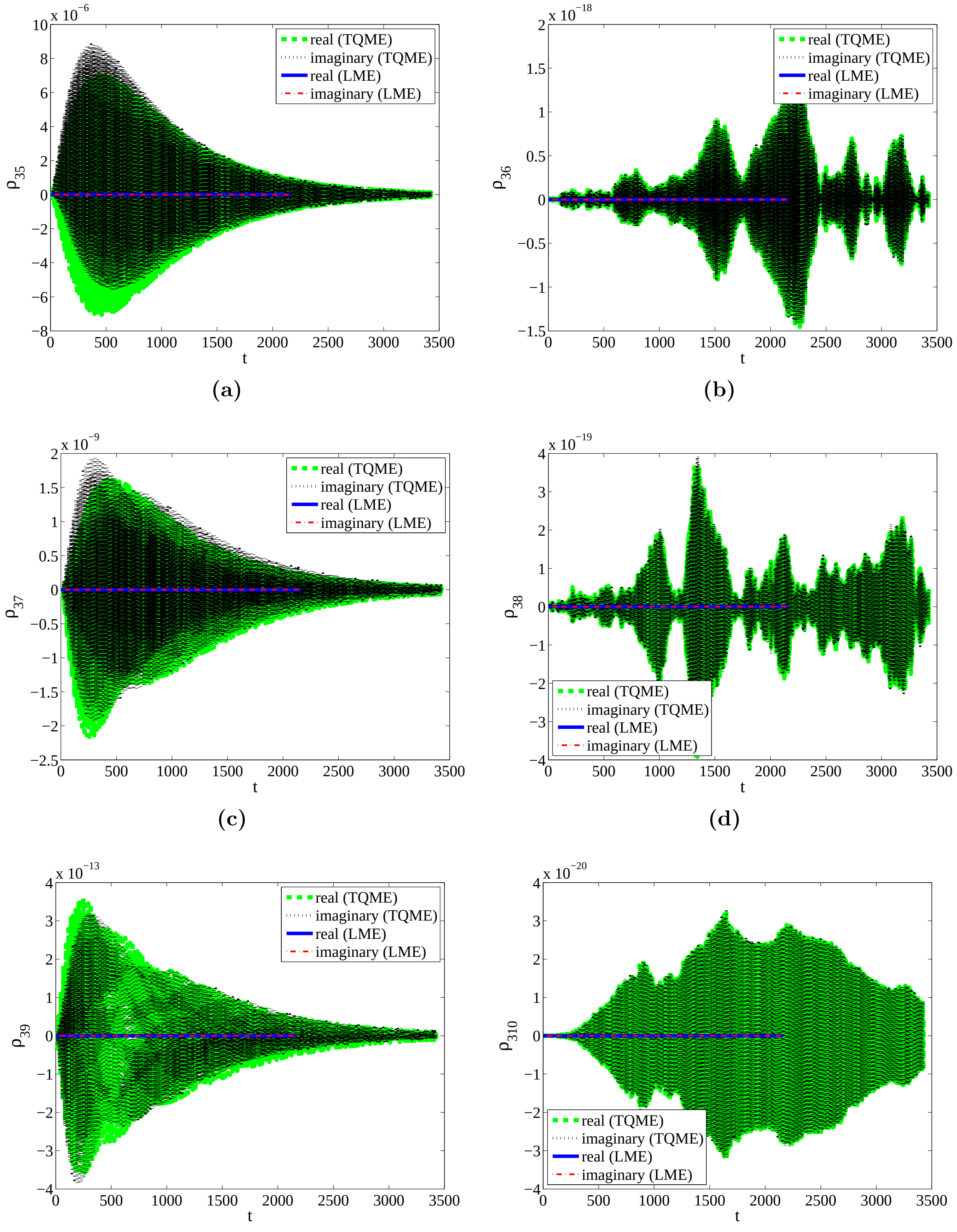


(a) (b)

(c) (d)

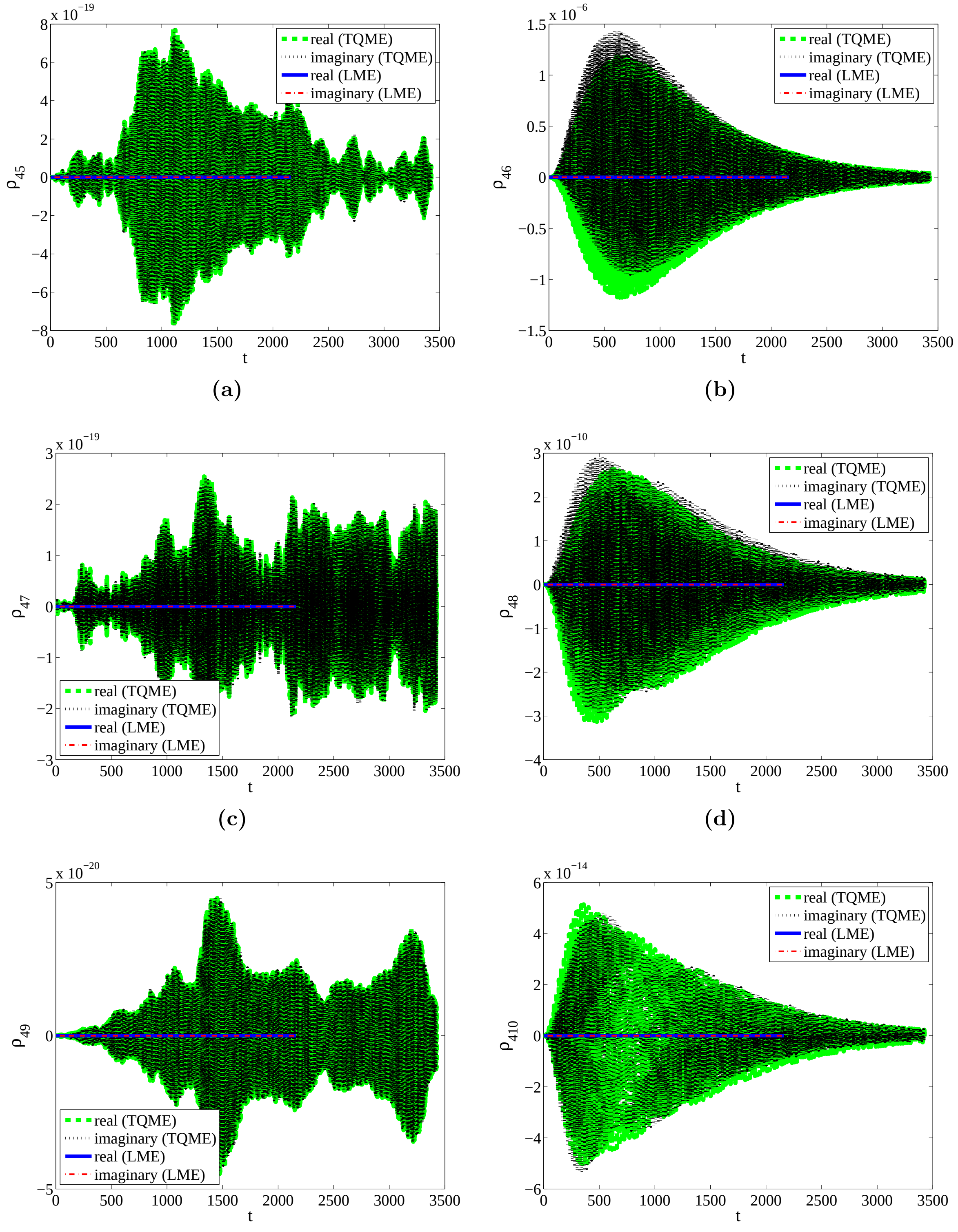
(e) (f)

Figure 10.3.1.11: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{26}, ρ_{27}, ρ_{28}, ρ_{29}, ρ_{210}, ρ_{34}.



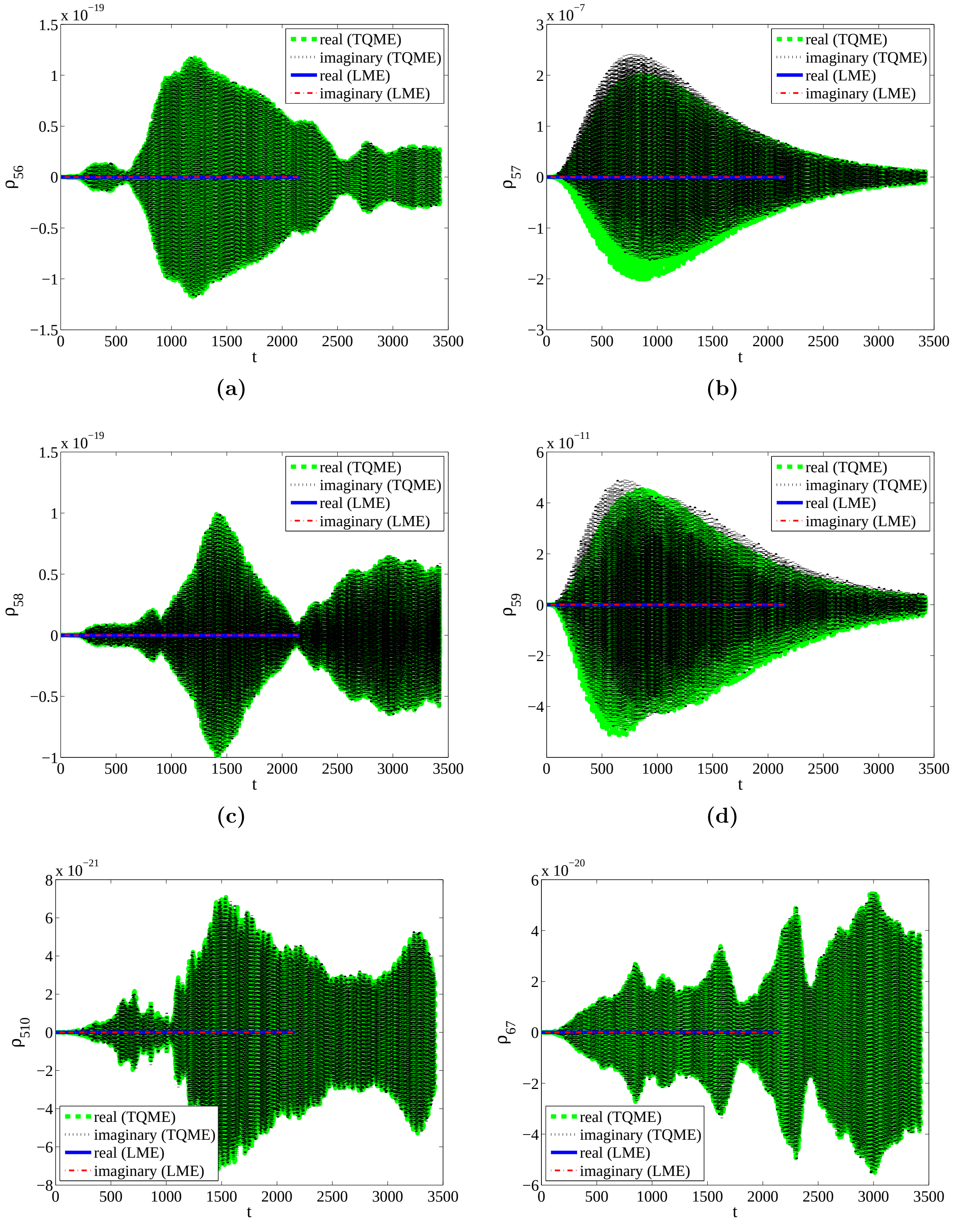
(a) (b) (c) (d) (e) (f)

Figure 10.3.1.12: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{35}, ρ_{36}, ρ_{37}, ρ_{38}, ρ_{39}, ρ_{310}.



(a) **(b)** **(c)** **(d)** **(e)** **(f)**

Figure 10.3.1.13: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{45}, ρ_{46}, ρ_{47}, ρ_{48}, ρ_{49}, ρ_{410}.

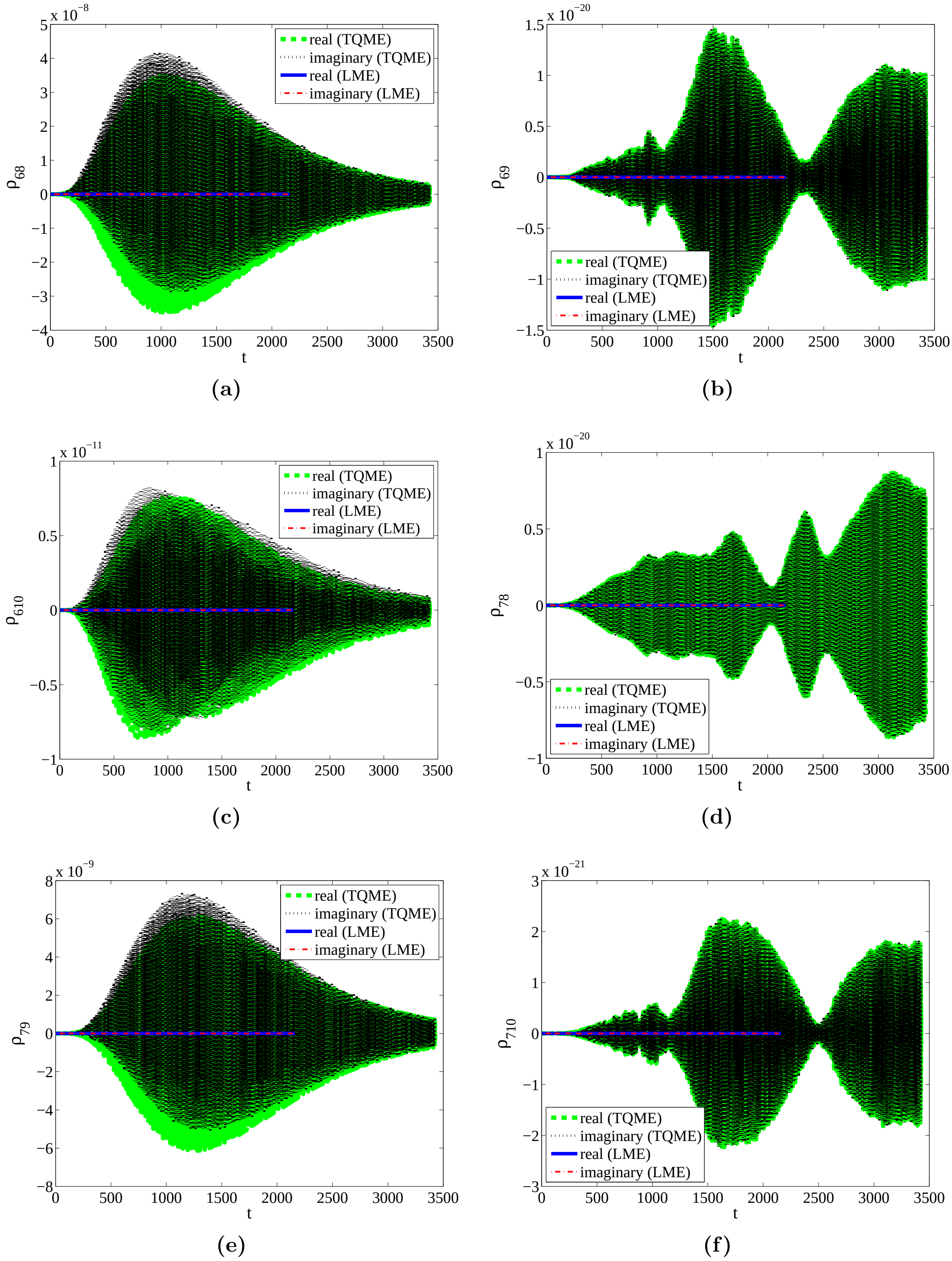


(a) (b)

(c) (d)

(e) (f)

Figure 10.3.1.14: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{56}, ρ_{57}, ρ_{58}, ρ_{59}, ρ_{510}, ρ_{67}.

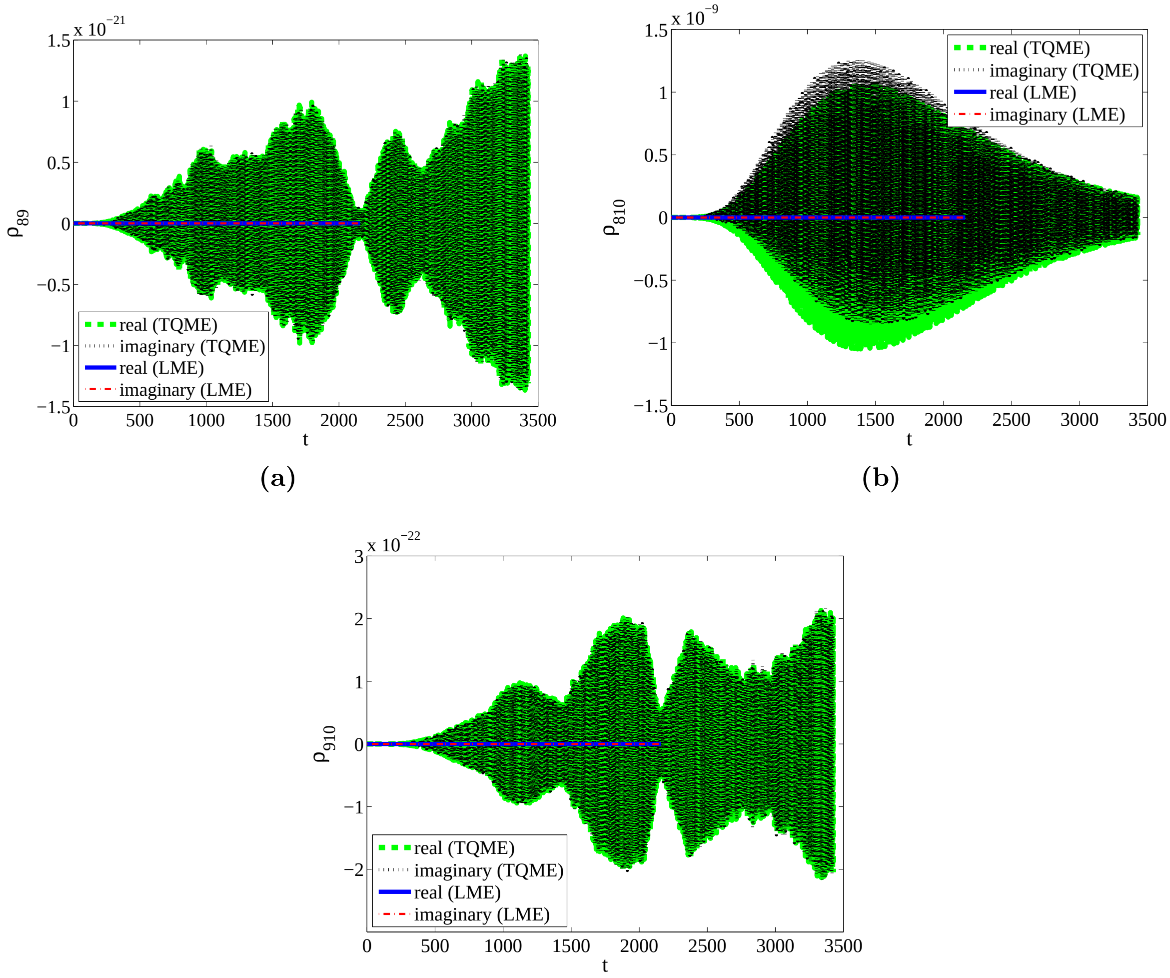


(a) **(b)**

(c) **(d)**

(e) **(f)**

Figure 10.3.1.15: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{68}, ρ_{69}, ρ_{610}, ρ_{78}, ρ_{79}, ρ_{710}.



(a)

(b)

(c)

Figure 10.3.1.16: Same as 10.3.1.7 but for the non-diagonal density matrix elements, ρ_{89}, ρ_{810}, ρ_{910}.

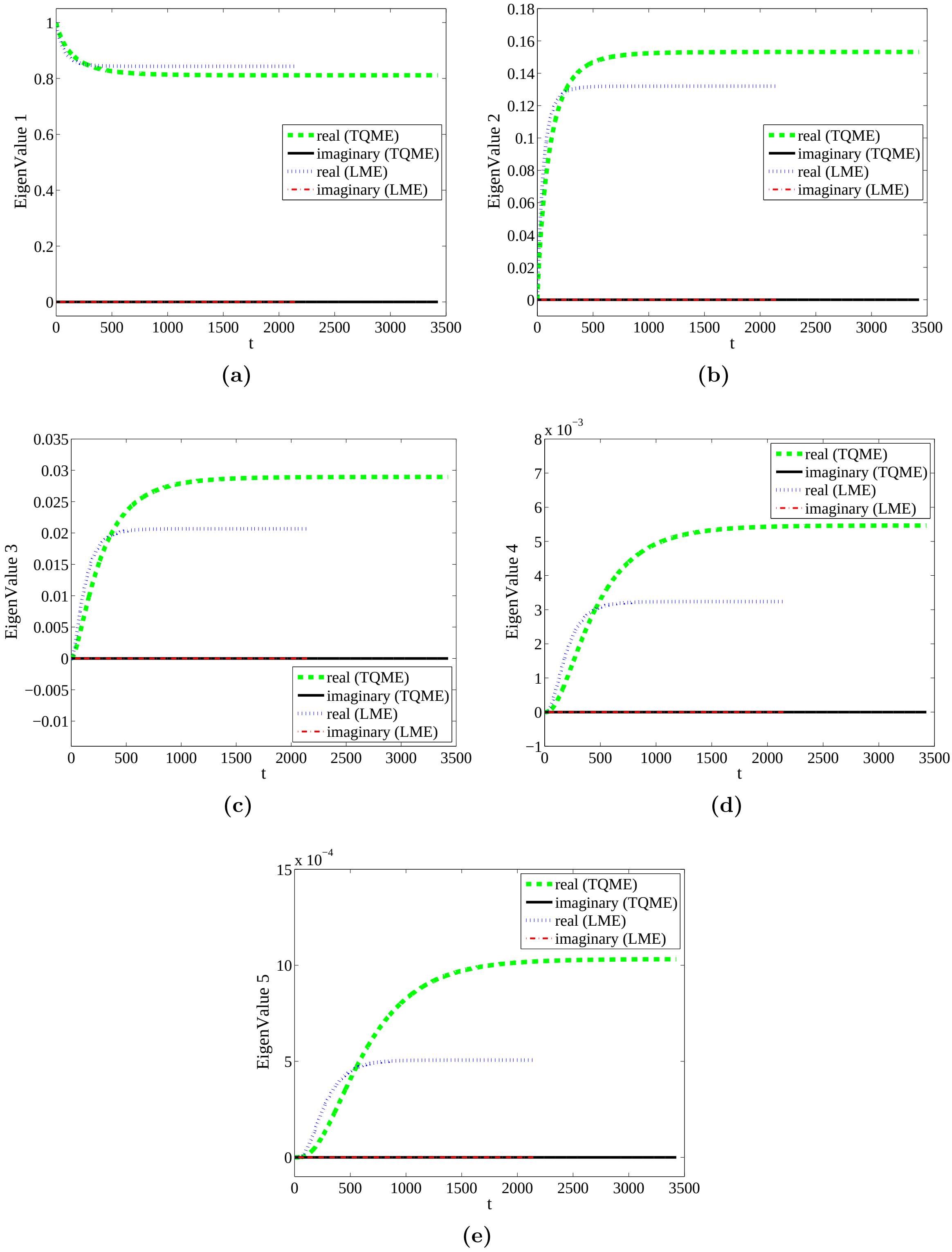
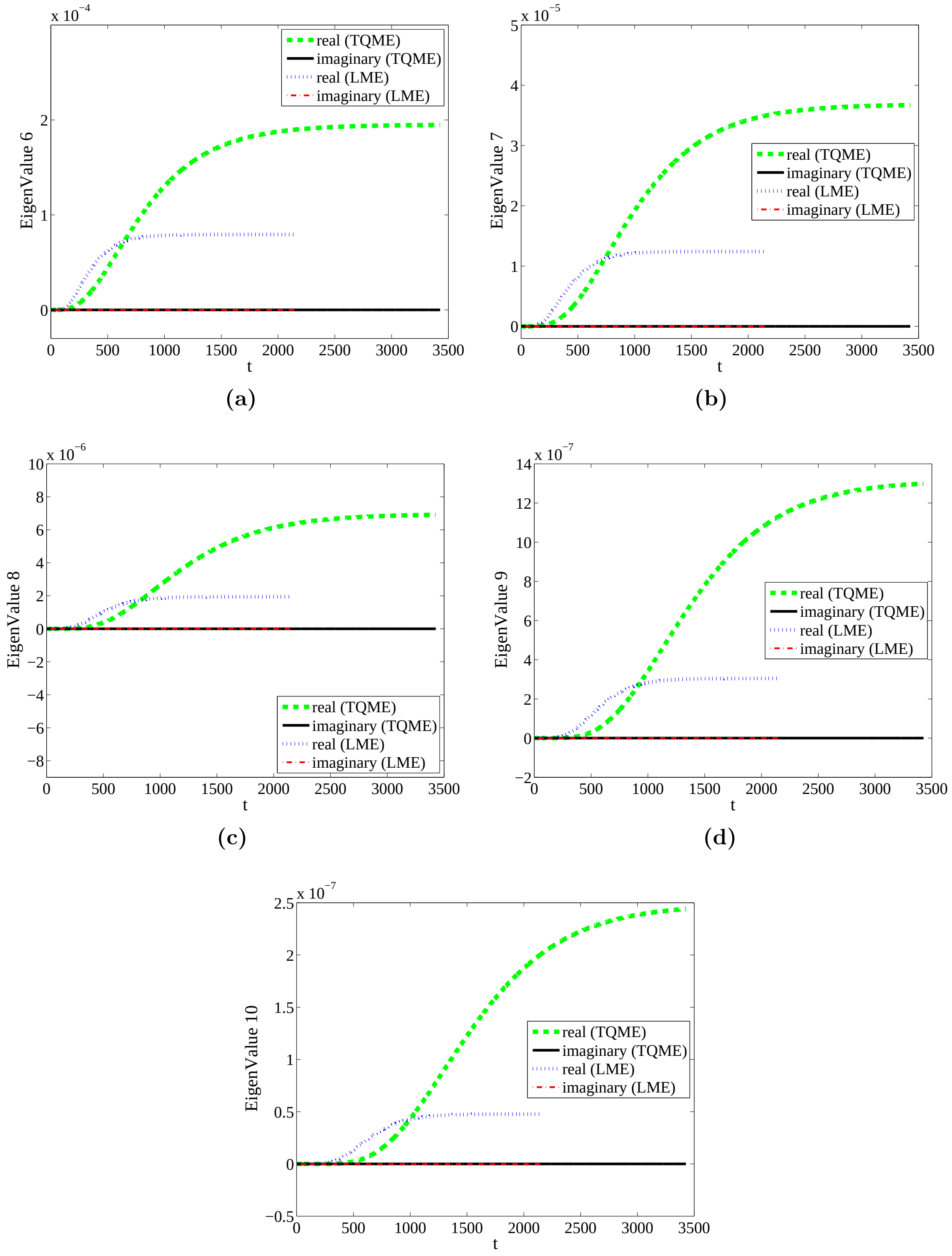


Figure 10.3.1.17: Same as 10.3.1.7 but for the first five eigenvalues of the density matrix.

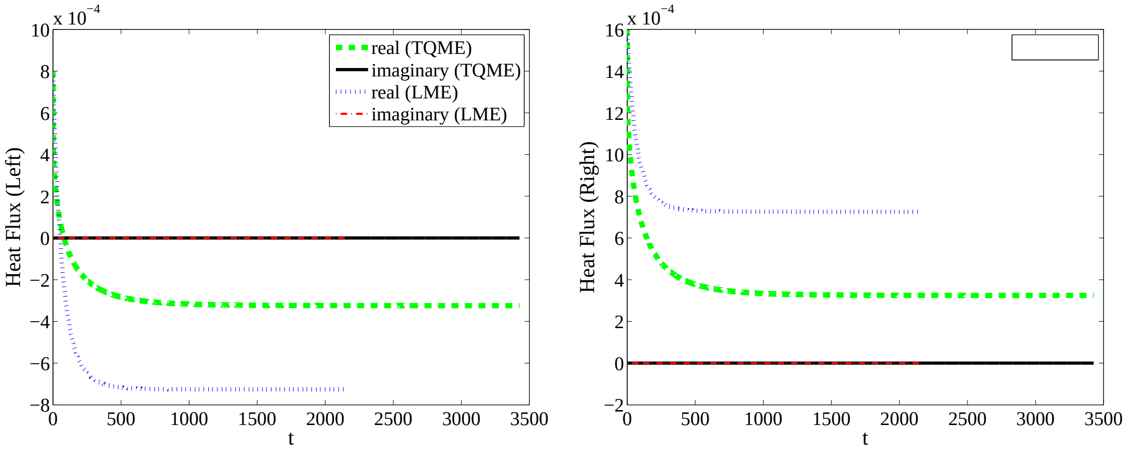


(a) **(b)**

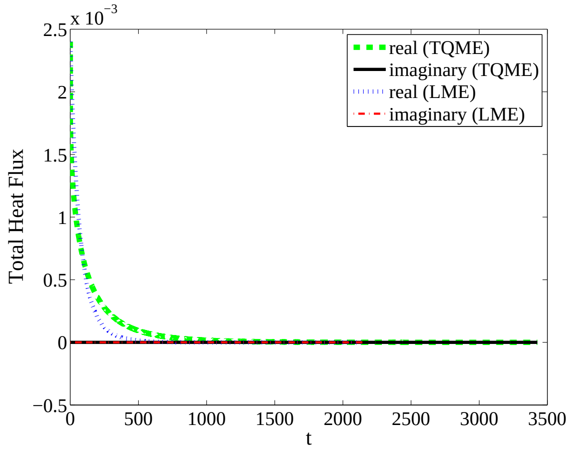
(c) **(d)**

(e)

Figure 10.3.1.18: Same as 10.3.1.7 but for the last five eigenvalues of the density matrix.



(a) **(b)**



(c)

Figure 10.3.1.19: Same as 10.3.1.7 but for the heat flux of the left (10.3.1.4a), right (10.2.1.4b) heat baths and the total one (10.3.1.4c).

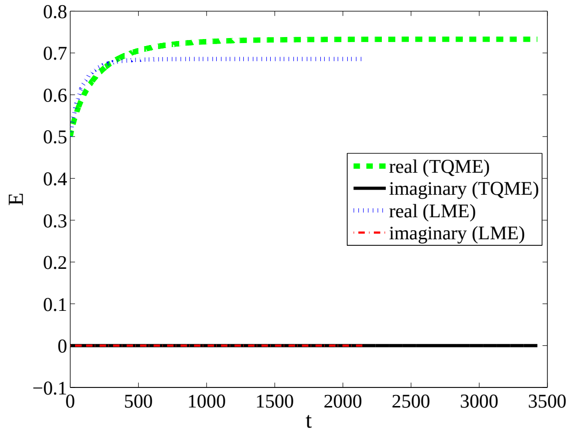
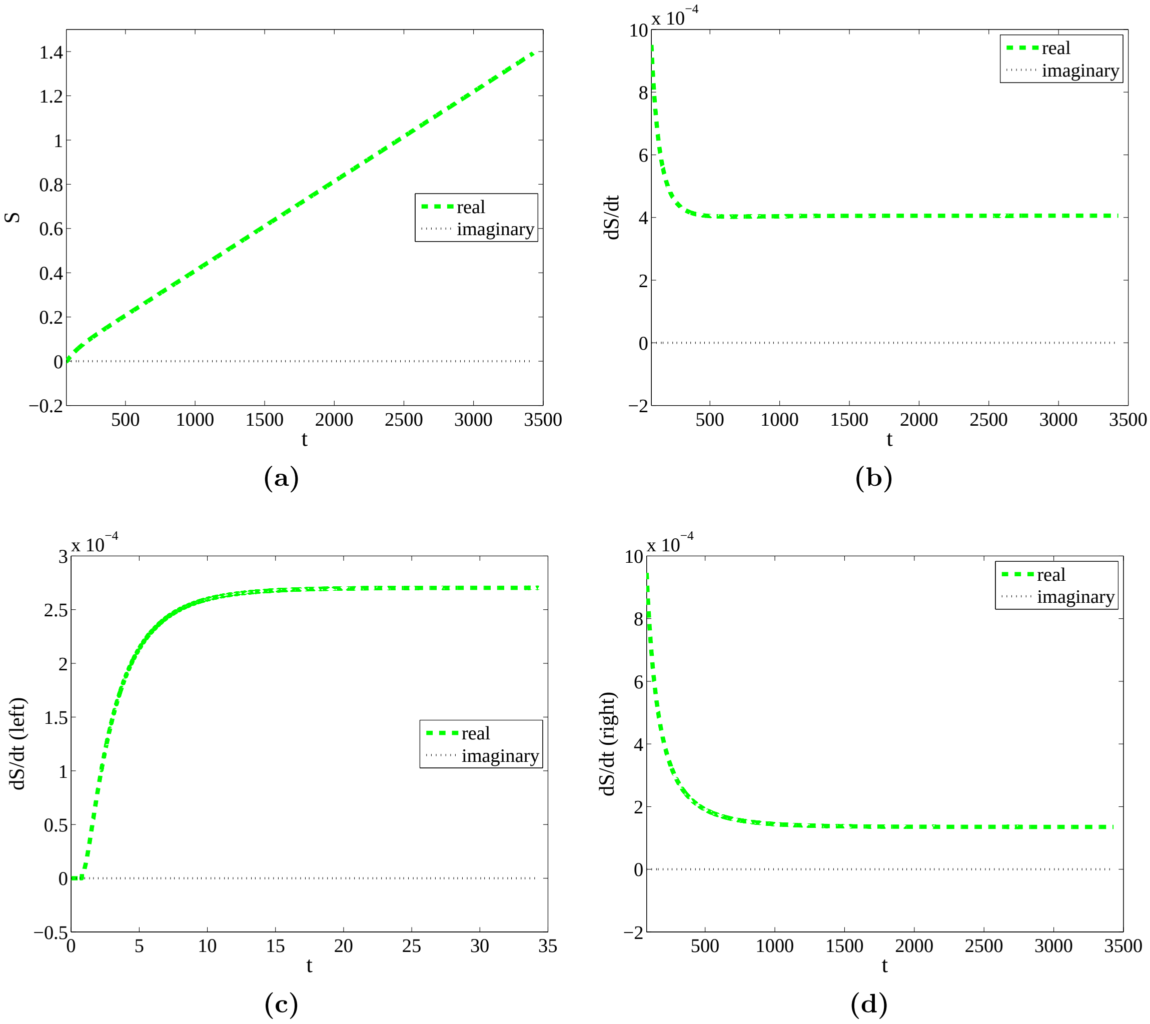


Figure 10.3.1.20: Same as 10.3.1.7 but for the energy E of the system.



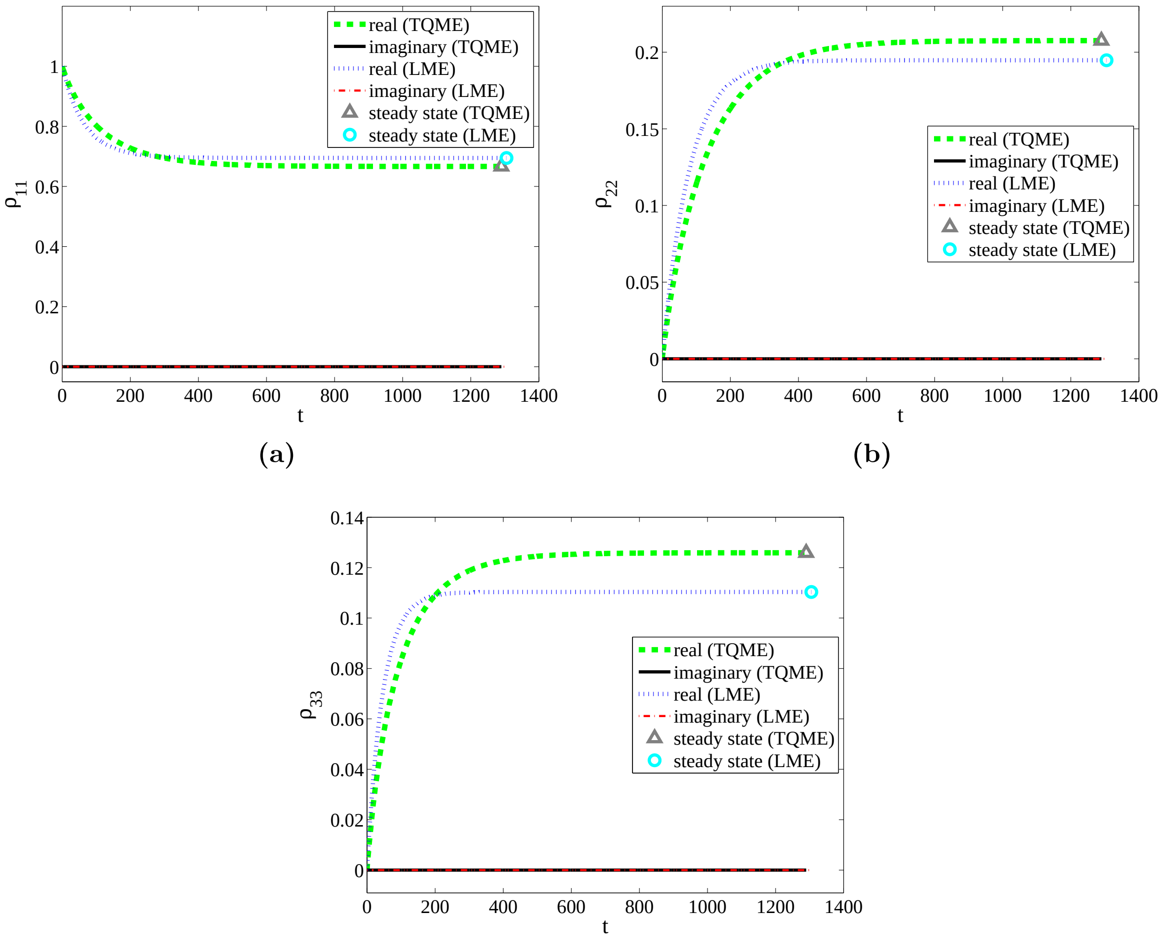
(a) (b) (c) (d)

Figure 10.3.1.21: Time evolution of the real and imaginary part of the entropy S of the system and $\frac{dS}{dt}$, $\frac{dS}{dt}$ (left), $\frac{dS}{dt}$ (right), using the Thermodynamic Quantum Master Equation (TQME) (real (green), imaginary (black)) for the case of the Harmonic Oscillator (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

10.3.2 Direct Steady-State Solution

In this section, we present the results obtained by an independent, non-linear matrix algebra solver that we implemented for computing the steady-state solution of the density matrix. These steady-state solutions are compared with the corresponding values taken from the dynamic relaxation of numerical integration for all the studied occasions.

Three-Level System (Qutrit)

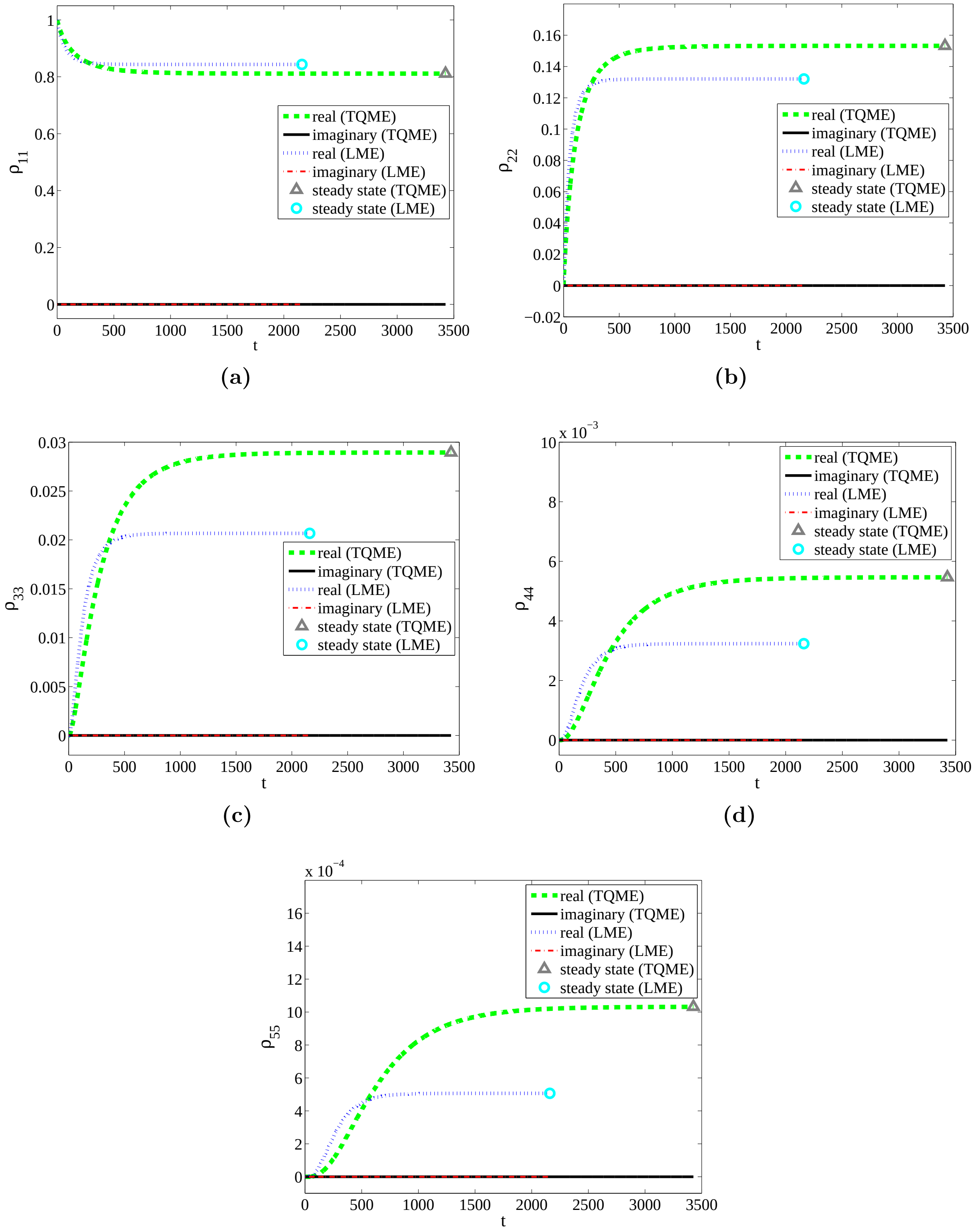


(a) **(b)**

(c)

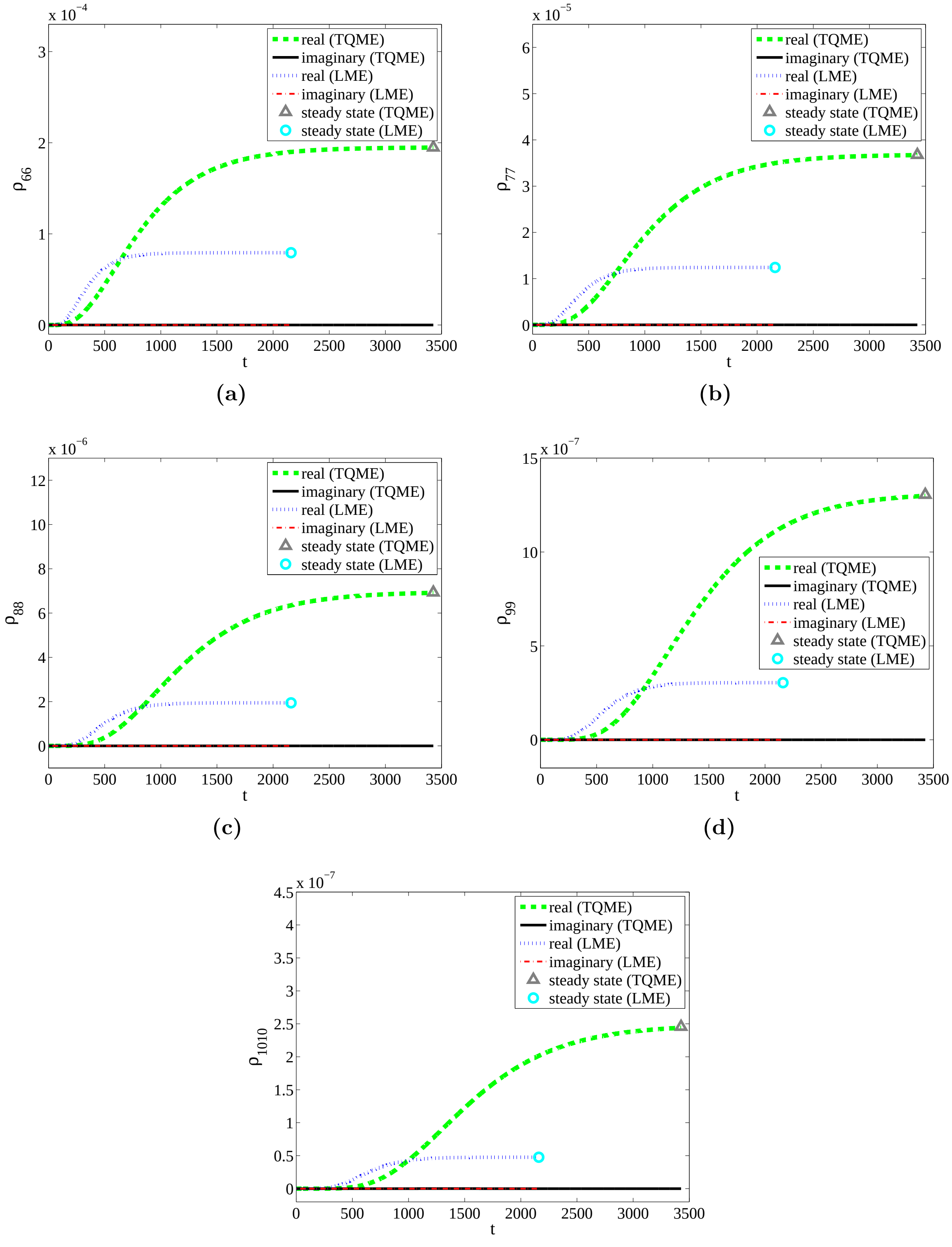
Figure 10.3.2.1: Comparison of the steady-state solution of the diagonal density matrix elements, $\rho_{11}, \rho_{22}, \rho_{33}$, between the time integration and the direct calculation of the steady-state values, using the Lindblad Master Equation (LME) (time integration: real (green), imaginary (black), steady-state solution: real (grey triangular)) and the Thermodynamic Quantum Master Equation (TQME) (time integration: real (blue), imaginary (red), steady-state solution: real (light blue circle)), in the case of the Three-Level system (Qutrit), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

Harmonic Oscillator (10 states)



(a) (b) (c) (d) (e)

Figure 10.3.2.2: Comparison of the steady-state solution of the diagonal density matrix elements, ρ_{11}, ρ_{22}, ρ_{33}, ρ_{44}, ρ_{55}, between the time integration and the direct calculation of the steady-state values, using the Lindblad Master Equation (LME) (time integration: real (green), imaginary (black), steady-state solution: real (grey triangular)) and the Thermodynamic Quantum Master Equation (TQME) (time integration: real (blue), imaginary (red), steady-state solution: real (light blue circle)), in the case of the Harmonic Oscillator (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.



(a)

(b)

(c)

(d)

(e)

Figure 10.3.2.3: Same as 10.3.2.2 but for ρ_{66}, ρ_{77}, ρ_{88}, ρ_{99}, ρ_{1010}.

10.3.3 Effective Temperatures

Here, we present the effective, steady-state temperature using Eq. 7.3.1 and the steady-state values of the diagonal elements of the density matrix, acquired from the direct steady-state solution in the previous section. The following results refer to both quantum systems, the three-level and the harmonic oscillator, using the Lindblad-type and the Thermodynamic Quantum Master Equation.

	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$
LME	0.6949	0.1947	0.1104
TQME	0.6665	0.2076	0.1259

Table 10.3.3.1: Steady-state solutions for the diagonal density matrix elements using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Three-Level system (Qutrit), with $T_l = 0.4$, $T_r = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

	T_{12}^{eff}	T_{23}^{eff}	T_{13}^{eff}
LME	0.5503	0.5280	0.5434
TQME	0.6000	0.6000	0.6000

Table 10.3.3.2: Effective steady-state temperatures using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Three-Level system (Qutrit), with $T_l = 0.4$, $T_r = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$	$\rho_{44,ss}$	$\rho_{55,ss}$
LME	0.8434	0.1320	0.0207	3.236E-03	5.066E-04
TQME	0.8111	0.1532	0.0289	0.0055	0.0010

Table 10.3.3.3: Steady-state solutions for the first five diagonal density matrix elements using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Harmonic Oscillator system (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

	$\rho_{66,ss}$	$\rho_{77,ss}$	$\rho_{88,ss}$	$\rho_{99,ss}$	$\rho_{1010,ss}$
LME	7.9E-05	1.2E-05	1.9E-06	3.0E-07	4.8E-08
TQME	0.0002	3.676E-05	6.9E-06	1.3E-06	2.5E-07

Table 10.3.3.4: Same as Table 10.3.3.3 for the last five diagonal density matrix elements.

	T_{ij}^{eff}, for $j > i,\ i, j = 1, \ldots, 10$
LME	0.5393
TQME	0.6000

Table 10.3.3.5: Effective steady-state temperatures using the Lindblad Master Equation (LME) and the Thermodynamic Quantum Master Equation (TQME), for the Harmonic Oscillator system (10 states), with $T_{e,l} = 0.4$, $T_{e,r} = 0.8$ and $\gamma_l = \gamma_r = 0.001$.

10.3.4 Parametric Analysis

In this section, we present steady-state results for the density matrix and the effective temperatures for a variety of temperature pairs acquired from the direct steady-state solver. These results refer to both quantum systems, the three-level and the harmonic oscillator, using the Lindblad-type and the Thermodynamic Quantum Master Equation.

$T_{e,l}$	$T_{e,r}$	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$
0.1	0.8	0.9916	0.0079	0.0004
0.2	0.8	0.8742	0.0977	0.0281
0.3	0.8	0.7611	0.1619	0.0770
0.4	0.8	0.6950	0.1947	0.1103
0.5	0.8	0.6540	0.2142	0.1318
0.6	0.8	0.6256	0.2273	0.1470
0.7	0.8	0.6042	0.2371	0.1587
0.8	0.8	0.5871	0.2447	0.1682
0.9	0.8	0.5726	0.2511	0.1763
1	0.8	0.5605	0.2563	0.1832

Table 10.3.4.1: Steady-state solutions for the diagonal density matrix elements, referring to the Three-Level system (Qutrit), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.001$.

$T_{e,l}$	$T_{e,r}$	T_{12}^{eff}	T_{23}^{eff}	T_{13}^{eff}
0.1	0.8	0.14	0.10	0.13
0.2	0.8	0.32	0.24	0.29
0.3	0.8	0.45	0.40	0.44
0.4	0.8	0.55	0.53	0.54
0.5	0.8	0.63	0.62	0.62
0.6	0.8	0.69	0.69	0.69
0.7	0.8	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85
1	0.8	0.89	0.89	0.89

Table 10.3.4.2: Effective steady-state temperatures, referring to the Three-Level system (Qutrit), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, $T_{e,l}$ and $T_{e,r}$, and $\gamma_l = \gamma_r = 0.001$.

T_l	T_r	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$
0.1	0.8	0.7579	0.1599	0.0821
0.2	0.8	0.7236	0.1784	0.0979
0.3	0.8	0.6933	0.1942	0.1125
0.4	0.8	0.6665	0.2076	0.1259
0.5	0.8	0.6429	0.2190	0.1380
0.6	0.8	0.6221	0.2289	0.1491
0.7	0.8	0.6036	0.2373	0.1591
0.8	0.8	0.5871	0.2447	0.1682
0.9	0.8	0.5723	0.2512	0.176
1	0.8	0.5591	0.2568	0.1840

Table 10.3.4.3: Steady-state solutions for the diagonal density matrix elements, referring to the Three-Level system (Qutrit), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.001$.

T_l	T_r	T_{12}^{eff}	T_{23}^{eff}	T_{13}^{eff}
0.1	0.8	0.45	0.45	0.45
0.2	0.8	0.50	0.50	0.50
0.3	0.8	0.55	0.55	0.55
0.4	0.8	0.60	0.60	0.60
0.5	0.8	0.65	0.65	0.65
0.6	0.8	0.70	0.70	0.70
0.7	0.8	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85
1	0.8	0.90	0.90	0.90

Table 10.3.4.4: Effective steady-state temperatures, referring to the Three-Level system (Qutrit), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, $T_{E,l}$ and $T_{e,r}$, and $\gamma_l = \gamma_r = 0.001$.

T_l	T_r	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$	$\rho_{44,ss}$	$\rho_{55,ss}$
0.1	0.8	0.9996	4.0791E-04	1.7E-07	6.8E-11	2.8E-14
0.2	0.8	0.9692	0.0298	0.000919012	2.82992E-05	8.7E-07
0.3	0.8	0.9018	0.0886	0.008696108	8.53947E-04	8.3857E-05
0.4	0.8	0.8434	0.1320	0.02067123	0.0032	5.0661E-04
0.5	0.8	0.7996	0.1602	0.032113877	0.0064	0.0013
0.6	0.8	0.7654	0.1795	0.042110026	0.0099	0.0023
0.7	0.8	0.7374	0.1936	0.050833087	0.0133	0.0035
0.8	0.8	0.7135	0.2044	0.058567457	0.0168	0.0048
0.9	0.8	0.69225	0.2131	0.065549415	0.0202	0.0062
1	0.8	0.6734	0.2199	0.07184711	0.0235	0.0077

Table 10.3.4.5: Steady-state solutions for the first five diagonal density matrix elements, referring to the Harmonic Oscillator system (10 states), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.001$.

T_l	T_r	$\rho_{66,ss}$	$\rho_{77,ss}$	$\rho_{88,ss}$	$\rho_{99,ss}$	$\rho_{1010,ss}$
0.1	0.8	1.1E-17	4.6E-21	1.9E-24	6.4E-28	3.1E-31
0.2	0.8	2.7E-08	8.3E-10	2.5E-11	7.8E-13	2.4E-14
0.3	0.8	8.2346E-06	8.1E-07	7.9E-08	7.8E-09	7.6E-10
0.4	0.8	7.931E-05	1.2415E-05	1.9E-06	3.0E-07	4.8E-08
0.5	0.8	2.5848E-04	5.1802E-05	1.0381E-05	2.1E-06	4.2E-07
0.6	0.8	5.4334E-04	1.2743E-04	2.9891E-05	7.0E-06	1.6E-06
0.7	0.8	9.2E-04	2.4154E-04	6.3418E-05	1.6650E-05	4.4E-06
0.8	0.8	0.0014	3.9462E-04	1.1306E-04	3.2393E-05	9.3E-06
0.9	0.8	0.0019	5.8700E-04	1.8057E-04	5.5550E-05	1.7088E-05
1	0.8	0.0025	8.1792E-04	2.6717E-04	8.7270E-05	2.8507E-05

Table 10.3.4.6: Same as Table 10.2.4.5 but for the last five diagonal density matrix elements.

$T_{e,l}$	$T_{e,r}$	T_{12}^{eff}	T_{23}^{eff}	T_{34}^{eff}	T_{45}^{eff}	T_{56}^{eff}
0.1	0.8	0.13	0.13	0.13	0.13	0.13
0.2	0.8	0.29	0.29	0.29	0.29	0.29
0.3	0.8	0.43	0.43	0.43	0.43	0.43
0.4	0.8	0.54	0.54	0.54	0.54	0.54
0.5	0.8	0.62	0.62	0.62	0.62	0.62
0.6	0.8	0.69	0.69	0.69	0.69	0.69
0.7	0.8	0.75	0.75	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85	0.85	0.85
1	0.8	0.89	0.89	0.89	0.89	0.89

Table 10.3.4.7: Effective steady-state temperatures for the first five transitions, referring to the Harmonic Oscillator system (10 states), using the Lindblad Master Equation (LME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.001$.

$T_{e,l}$	$T_{e,r}$	T_{67}^{eff}	T_{78}^{eff}	T_{89}^{eff}	T_{910}^{eff}
0.1	0.8	0.13	0.13	0.13	0.13
0.2	0.8	0.29	0.29	0.29	0.29
0.3	0.8	0.43	0.43	0.43	0.43
0.4	0.8	0.54	0.54	0.54	0.54
0.5	0.8	0.62	0.62	0.62	0.62
0.6	0.8	0.69	0.69	0.69	0.69
0.7	0.8	0.77	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85	0.85
1	0.8	0.89	0.89	0.89	0.89

Table 10.3.4.8: Same as 10.3.4.7 for the last four transitions.

$T_{e,l}$	$T_{e,r}$	$\rho_{11,ss}$	$\rho_{22,ss}$	$\rho_{33,ss}$	$\rho_{44,ss}$	$\rho_{55,ss}$
0.1	0.8	0.8916	0.0966	0.0105	0.0011	1.2297E-04
0.2	0.8	0.8647	0.1170	0.0158	0.0021	2.9006E-04
0.3	0.8	0.8377	0.1360	0.0221	0.0036	5.8153E-04
0.4	0.8	0.8111	0.1532	0.0289	0.0055	0.0010
0.5	0.8	0.7857	0.1684	0.0361	0.0077	0.0016
0.6	0.8	0.7603	0.1822	0.0437	0.0105	0.0025
0.7	0.8	0.7364	0.1941	0.0511	0.0135	0.0035
0.8	0.8	0.7135	0.2044	0.0586	0.0168	0.0048
0.9	0.8	0.6916	0.2133	0.0658	0.0203	0.0062
1	0.8	0.6708	0.2208	0.0727	0.0239	0.0079

Table 10.3.4.9: Steady-state solutions for the first five diagonal density matrix elements, referring to the Harmonic Oscillator system (10 states), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, $T_{e,l}$ and $T_{e,r}$, and $\gamma_l = \gamma_r = 0.001$.

$T_{e,l}$	$T_{e,r}$	$\rho_{66,ss}$	$\rho_{77,ss}$	$\rho_{88,ss}$	$\rho_{99,ss}$	$\rho_{1010,ss}$
0.1	0.8	1.3326E-05	1.4E-06	1.6E-07	1.7E-08	1.8E-09
0.2	0.8	3.9256E-05	5.3E-06	7.2E-07	9.7E-08	1.3E-08
0.3	0.8	9.4394E-05	1.5322E-05	2.5E-06	4.0E-07	6.5E-08
0.4	0.8	1.94859E-04	3.6769E-05	6.9E-06	1.3E-06	2.4E-07
0.5	0.8	3.5366E-04	7.5524E-05	1.6097E-05	3.4E-06	7.3E-07
0.6	0.8	6.0105E-04	1.4404E-04	3.4520E-05	8.3E-06	2.0E-06
0.7	0.8	9.3717E-04	2.4704E-04	6.5118E-05	1.7165E-05	4.52E-06
0.8	0.8	0.0014	3.9462E-04	1.1306E-04	3.2393E-05	9.3E-06
0.9	0.8	0.0019	5.9466E-04	1.8344E-04	5.6546E-05	1.7437E-05
1	0.8	0.0026	8.5370E-04	2.8103E-04	9.2514E-05	3.0455E-05

Table 10.3.4.10: Same as Table 10.3.4.9 but for the last five diagonal density matrix elements.

T_l	T_r	T_{12}^{eff}	T_{23}^{eff}	T_{34}^{eff}	T_{45}^{eff}	T_{56}^{eff}
0.1	0.8	0.45	0.45	0.45	0.45	0.45
0.2	0.8	0.50	0.50	0.50	0.50	0.50
0.3	0.8	0.55	0.55	0.55	0.55	0.55
0.4	0.8	0.60	0.60	0.60	0.60	0.55
0.5	0.8	0.65	0.65	0.65	0.65	0.65
0.6	0.8	0.70	0.70	0.70	0.70	0.70
0.7	0.8	0.75	0.75	0.75	0.75	0.75
0.8	0.8	0.80	0.80	0.80	0.80	0.80
0.9	0.8	0.85	0.85	0.85	0.85	0.85
1	0.8	0.90	0.90	0.90	0.90	0.90

Table 10.3.4.11: Effective steady-state temperatures for the first five transitions, referring to the Harmonic Oscillator system (10 states), using the Thermodynamic Quantum Master Equation (TQME) for several values of the heat bath temperatures, T_l and T_r, and $\gamma_l = \gamma_r = 0.001$.

T_l	T_r	T_{67}^{eff}	T_{78}^{eff}	T_{89}^{eff}	T_{910}^{eff}
0.1	0.8	0.450000014	0.450000018	0.45000002	0.450000022
0.2	0.8	0.500000002	0.500000002	0.500000002	0.500000002
0.3	0.8	0.549999739	0.54999976	0.549999762	0.549999762
0.4	0.8	0.599653821	0.599305437	0.598831861	0.598663963
0.5	0.8	0.647713735	0.646896873	0.645945614	0.645631154
0.6	0.8	0.7	0.700000001	0.700000001	0.700000001
0.7	0.8	0.749999999	0.749999999	0.75	0.750000001
0.8	0.8	0.799999744	0.799999744	0.799999745	0.799999746
0.9	0.8	0.850000004	0.850000005	0.850000007	0.850000008
1	0.8	0.900000005	0.900000006	0.900000008	0.90000001

Table 10.3.4.12: Same as Table 10.3.4.11 but for the last four transitions.

CHAPTER 11

DISCUSSION

In the previous section, we presented our results concerning a three-level system (qutrit) and a harmonic oscillator (of ten states), coupled with two heat baths of different temperatures, using the Lindblad-type of equation, Eq. 7.1.2, and the thermodynamic quantum master equation, 7.2.4.1. The solutions refer to the time-integration of the above equation, using a fourth order Adams-Bashforth integration scheme with the help of a single-step Euler scheme for the starting values, and to an independent, non-linear matrix algebra solver for computing the steady-state solution of the density matrix using the Newton-Raphson method.

To begin with, the Lindblad master equation is linear while the thermodynamic one is strongly non-linear. The coupling constants have been chosen so that in the special case of interaction with one heat bath, both lead to the same final (Gibbs) steady-state, Figs 10.1.1.1, 10.1.1.6 - 10.1.1.7. In the case where the quantum system is coupled with two heat baths, the results in each set for the diagonal components are different. Also the dynamics is diferent; non-diagonal terms go to zero but by taking in-between non-zero values, Fig. 10.2.1.2, 10.2.1.9 - 10.2.1.16. In addition to this case, we observe that the steady-state values of the two sets, where all inputs are the same except from γ_k $(k = l, r)$, they differ only in the relaxation time. More analytically, in set 2, where γ_k is smaller, the time distance to equilibrium is larger.

Another point is that the eigenvalues in all the cases of interest, as well as the diagonal elements of the density matrix, are real and positive and the sum of the latter terms is equal to one during the simulation process, Figs. 10.2.1.3, 10.1.1.3, 10.1.1.16 - 10.1.1.17, 10.2.1.3, 10.2.1.3, 10.2.1.17 - 10.2.1.18, 10.3.1.3, 10.3.1.3, 10.3.1.17 - 10.3.1.18. These results ensures that the calculations are performed in the right manner, preserving the properties of the density matrix.

Furthermore, we can observe in Figs. 10.1.1.4a, 10.1.1.18a, 10.2.1.4c, 10.2.1.19c, 10.3.1.4c, 10.3.1.19c that the total heat flux We have verified that the total heat flux is driven to zero, as we expected. This exact result verifies the consistency check that we mentioned earlier and shows that the amount of heat flux coming from the heat bath with higher temperature value (right) towards the quantum subsystem is equal to the amount of heat flux exiting from it, towards the heat bath with the lower temperature (left). One more observation is that the individual heat fluxes, coming in or out, are of opposite sign, as shown in Figs. 10.2.1.4a, 10.2.1.4b, 10.2.1.19a, 10.2.1.19b, 10.3.1.4a, 10.3.1.19a, 10.3.1.4b, 10.3.1.19b.

Also, another observation is that the entropy of the composite system (quantum system and environment), in the case of the thermodynamic quantum master equation for both examining systems, Figs. 10.2.1.6,10.2.1 10.3.1.6,10.3.1, increases continuously with time as heat flows from the hot to cold environment through the quantum subsystem. At steady state the term $\frac{dS}{dt}$ attains a constant (but non-zero) value.

Finally, the steady-state values obtained from the time integration and the direct, algebraic solution are in a very good agreement, according to Figs. 10.1.2.1 - 10.1.2.3, 10.2.2.1 - 10.2.2.3, 10.3.2.1 - 10.3.2.3. This result allows us to study the response of the quantum system coupled with the two heat baths for several values of the two bath temperatures, and friction coefficients.

Chapter 12

Electromagnetically Induced Transparency (EIT)

12.1 Introduction

Coherent preparation by laser light of quantum states of atoms and molecules can lead to quantum interference in the amplitudes of optical transitions. Electromagnetically induced transparency (EIT) is a quantum interference phenomenon that arises when coherent optical fields couple to the states of a material quantum system. In EIT the interference occurs between alternative transition pathways, driven by radiation fields within the internal states of the quantum system. Interference effects arise, because in quantum mechanics the probability amplitudes (which may be positive or negative in sign), rather than probabilities, must be summed and squared to obtain the total transition probability between the relevant quantum states. Interference between the amplitudes may lead to either an enhancement (constructive interference) or a complete cancellation (destructive interference) in the total transition probability. As a consequence, interference effects can lead to profound modification of the optical and nonlinear optical properties of a medium. Thus, control of optical or nonlinear optical properties and processes becomes possible.

The cause of the modified optical response of an atomic medium in this case is the laser-induced coherence of atomic states, which leads to quantum interference between the excitation pathways that control the optical response. We can in this way eliminate the absorption and refraction (linear susceptibility) at the resonant frequency of a transition. This was termed electromagnetically induced transparency (EIT) by Harris and co-workers [35] in 1990. The importance of EIT stems from the fact that it gives rise to greatly enhanced nonlinear susceptibility in the spectral region of induced transparency of the medium and is associated with steep dispersion. The first experimental observation of this effect was demonstrated by Boller et al. [36] in Strontium (Sr) vapour, in 1991.

EIT is achievable only in atoms with specific energy structures. For a three level system, EIT requires two dipole allowed transitions ($|1\rangle \rightarrow |3\rangle$ and $|2\rangle \rightarrow |3\rangle$) and one forbidden transition ($|1\rangle \rightarrow |2\rangle$ is dipole forbidden). A strong laser, what we term the control laser, is tuned to the resonant frequency of the upper two levels. Then, a weak probe laser is scanned in frequency across the other transition. The medium is observed to have the properties plotted in Fig. 12.1.1 in response to the probe beam.

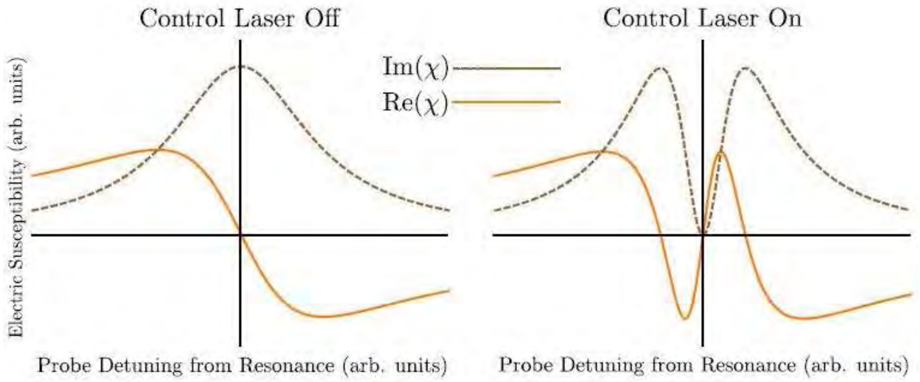


Figure 12.1.1: Simple EIT Plot. Here we are plotting the real and imaginary components of the complex linear susceptibility. The imaginary component corresponds to absorption - on the left we see a typical Lorentzian absorption peak while the control laser is inactive. When the control laser is applied, the absorption peak splits revealing a transparency at what was the maximal absorption. The real components appear in the dispersion relation, relating wave speed to frequency. [3]

The most interesting effect of EIT is not the transparency itself - this level of transparency could be achieved by tuning our laser away from the atomic resonance. What is particularly interesting is that EIT also induces large dispersion effects at the atomic resonance. In particular, a very steep linear dispersion relation is found at the point of minimal absorption.

There are three energy level configurations for three level atoms that can demonstrate EIT, shown in Fig. 12.1.2. While all three systems demonstrate EIT, we will be deriving EIT for a three level Λ-atom, as the effects are diminished in cascade (Ξ) and V systems due to high decay rates from $|2\rangle$, which shortens the coherence lifetime. The Λ-atom's $|2\rangle$ state is a metastable state with greatly reduced decays and longer coherence lifetimes. We are ultimately interested in the optical properties of the medium, specifically the dispersion and absorption of the probe laser. These characteristics are described to first order by the frequency dependent complex valued linear electric susceptibility χ, which is defined by

$$\boldsymbol{P} = \epsilon_0 \chi \boldsymbol{E} \tag{12.1.1}$$

where $\boldsymbol{P}$ is the dielectric polarization of the medium, $\boldsymbol{E}$ is the electric field, and ϵ_0 is the permittivity of free space. Knowledge of χ completely determines the material properties we are seeking. Note that $\boldsymbol{P}$, $\boldsymbol{E}$ and χ are all macroscopic quantities. However, in order to find χ, we need to consider individual atoms.

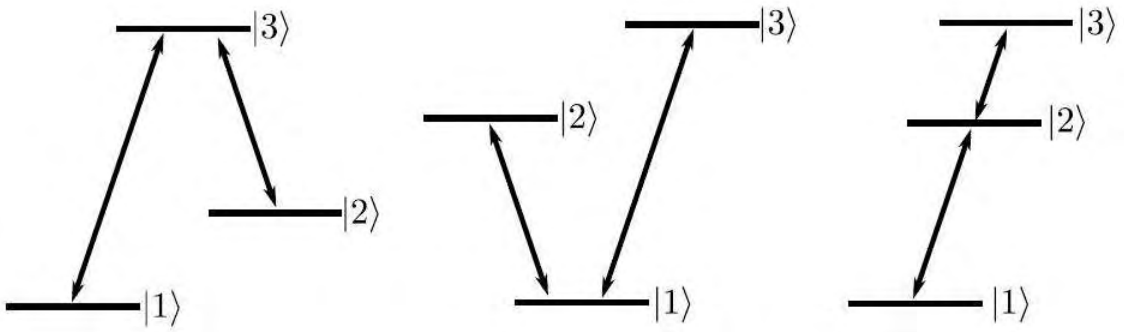


Figure 12.1.2: EIT capable systems. All three level systems capable of demonstrating EIT have one of three possible energy level structures: Λ type, V type, and cascade or Ξ type. Each has two dipole allowed transitions and one dipole forbidden transition, with the only difference being the relative arrangement of the energy levels. [3]

In the following section, we present the procedure followed in order to calculate the susceptibility of a medium, for two different master equations. Our approach is based on [3].

12.2 Derivation of H_{EIT}

The system under investigation is a three level Λ atom, consisting of the eigenstates $|1\rangle$, $|2\rangle$ and $|3\rangle$, with corresponding eigenvalue energies $\hbar\omega_n$. We have labelled the states in order of increasing energy, where $|1\rangle$ is a stable ground state, $|2\rangle$ is a metastable state, and both are coupled to the excited state $|3\rangle$.

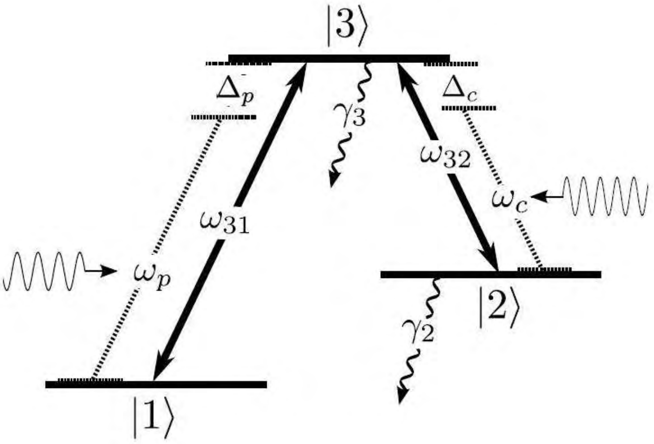


Figure 12.2.1: Lambda atom with detunings and decay. States $|1\rangle \rightarrow |3\rangle$ are resonant with frequency $\omega_{31} = \omega_3 - \omega_1$, states $|2\rangle \rightarrow |3\rangle$ are resonant with frequency $\omega_{32} = \omega_3 - \omega_2$. These transitions are driven, respectively, with a probe laser of frequency ω_p and control laser of frequency ω_c. The probe laser is detuned from resonance by $\Delta_p = \omega_p - \omega_{31}$, while the control laser is detuned from resonance by $\Delta_c = \omega_c - \omega_{32}$. The upper states have a decay rate γ_3 and γ_2, while the ground state is stable. The transition $|1\rangle \rightarrow |2\rangle$ is dipole forbidden, resulting in a very small γ_2 ($|2\rangle$ is a metastable state). [3]

The first step is to describe how the quantum mechanical atom behaves in the applied field. For this it is constructed a Hamiltonian (H_0) describing the three level atom, and approximate the field's effects as a dipole perturbation (H_1), which is given as the energy of the dipole moment operator ($\wp$).

$$H_0 = \left(\sum_n |n\rangle\langle n|\right) H \left(\sum_n |n\rangle\langle n|\right) = \begin{pmatrix} \hbar\omega_1 & 0 & 0 \\ 0 & \hbar\omega_2 & 0 \\ 0 & 0 & \hbar\omega_3 \end{pmatrix} \tag{12.2.1}$$

The $|2\rangle \rightarrow |3\rangle$ transition is driven by a strong control field of amplitude $\boldsymbol{\mathcal{E}}_c$ and frequency ω_c, while the $|1\rangle \rightarrow |3\rangle$ transition is driven by a weak probe field of amplitude $\boldsymbol{\mathcal{E}}_p$ and frequency ω_p. All other energy levels are assumed to be sufficiently off resonance for other transitions to be negligible.The applied field can be written as

$$\boldsymbol{E} = \boldsymbol{\mathcal{E}}_p cos(\omega_p t - \boldsymbol{k}_p \cdot \boldsymbol{r}) + \boldsymbol{\mathcal{E}}_c cos(\omega_c t - \boldsymbol{k}_c \cdot \boldsymbol{r}), \tag{12.2.2}$$

where $\boldsymbol{k}$ are the wave vectors associated with ω. For incident light with wavelengths much longer than the effective radius of the atom, $\lambda >> r$, the spatial component can be dropped and electric field, Eq. 12.2.2 becomes

$$\begin{aligned} \boldsymbol{E} &= \boldsymbol{\mathcal{E}}_p cos(\omega_p t) + \boldsymbol{\mathcal{E}}_c cos(\omega_c t) \\ &= \boldsymbol{\mathcal{E}}_p \frac{1}{2}\left(e^{i\omega_p t} + e^{-i\omega_p t}\right) + \boldsymbol{\mathcal{E}}_c \frac{1}{2}\left(e^{i\omega_c t} + e^{-i\omega_c t}\right) \end{aligned} \tag{12.2.3}$$

The energy of this perturbation will be given by

$$H_1 = -q\boldsymbol{E} \cdot \hat{\boldsymbol{r}}, \tag{12.2.4}$$

where q is the electron charge, $\boldsymbol{E}$ is the classical vector valued electric field and $\hat{\boldsymbol{r}}$ is the position operator.The term $-q\boldsymbol{E} \cdot \hat{\boldsymbol{r}}$ is simply the energy associated with a dipole of charge q and separation vector $\hat{\boldsymbol{r}}$ in the applied field E. Thus, the assumption $\lambda >> r$ is known as the dipole approximation. Assuming the dipole is aligned with the electric field we have

$$H_1 = -qE \cdot \hat{r}. \tag{12.2.5}$$

The dipole operator is defined as $\wp = q\hat{r}$, and the elements of the operator in the eigenbasis of H_0 by $\wp_{nm} = \wp^*_{mn} = \langle n \,|\, \wp \,|\, m\rangle$. The perturbation becomes

$$H_I = -\wp E = -\left(\sum_n |n\rangle\langle n|\right) wp \left(\sum_n |n\rangle\langle n|\right) E = -E \begin{pmatrix} \wp_{11} & \wp_{12} & \wp_{13} \\ \wp_{21} & \wp_{22} & \wp_{23} \\ \wp_{31} & \wp_{32} & \wp_{33} \end{pmatrix} \tag{12.2.6}$$

To simplify the dipole moment operator, we assume $\wp_{12} = \wp_{21} = 0$, consistent with the forbidden $|1\rangle \rightarrow |2\rangle$ transition. Additionally we assume $\wp_{ii} = 0$, removing all the diagonal elements. This amounts to assuming that the atoms have no permanent dipole moments, which is true for atoms with spherically symmetric wavefunctions. So, we get that

$$H_I = -E \begin{pmatrix} 0 & 0 & \wp_{13} \\ 0 & 0 & \wp_{23} \\ \wp_{31} & \wp_{32} & 0 \end{pmatrix} \tag{12.2.7}$$

The full Hamiltonian, $H = H_0 + H_I$, can be massaged with some approximations and transformations to a more agreeable form, what we term the EIT Hamiltonian (H_{EIT}). To find this Hamiltonian, the Rotating Wave Approximation (RWA) is used, which neglects any rapidly oscillating terms (i.e., exponentials with large-valued superscripts) in the Hamiltonian. To reveal these terms, transformation of the Hamiltonian into the interaction picture is required using the time evolution operator

$$U(t) = e^{\frac{iH_0 t}{\hbar}} = \begin{pmatrix} e^{i\omega_1 t} & 0 & 0 \\ 0 & e^{i\omega_2 t} & 0 \\ 0 & 0 & e^{i\omega_1 t} \end{pmatrix} \tag{12.2.8}$$

Applying this transformation to H_1 (H_0 remains unaffected), as $UH_IU^\dagger$ we get that

$$UH_IU^\dagger = -E \begin{pmatrix} 0 & 0 & \wp_{13}e^{i(\omega_1-\omega_3)t} \\ 0 & 0 & \wp_{23}e^{i(\omega_2-\omega_3)t} \\ \wp_{13}e^{-i(\omega_1-\omega_3)t} & \wp_{23}e^{-i(\omega_2-\omega_3)t} & . \end{pmatrix} \tag{12.2.9}$$

Substituting the electric field and expanding the cosines in terms of exponentials, as below

$$\begin{aligned} \boldsymbol{E} &= -\boldsymbol{\mathcal{E}}_p cos(\omega_p t) + \mathcal{E}_c cos(\omega_c t) \\ &= \boldsymbol{\mathcal{E}}_p \frac{1}{2}\left(e^{i\omega_p t} + e^{-i\omega_p t}\right) + \mathcal{E}_c \frac{1}{2}\left(e^{i\omega_c t} + e^{-i\omega_c t}\right) \end{aligned} \tag{12.2.10}$$

we get

$$(UH_IU^\dagger)_{13} = -\left(\boldsymbol{\mathcal{E}}_p \frac{1}{2}\left(e^{i\omega_p t} + e^{-i\omega_p t}\right) + \mathcal{E}_c \frac{1}{2}\left(e^{i\omega_c t} + e^{-i\omega_c t}\right)\right)\wp_{13}e^{i(\omega_1-\omega_3)t} \tag{12.2.11a}$$

$$(UH_IU^\dagger)_{31} = -\left(\boldsymbol{\mathcal{E}}_p \frac{1}{2}\left(e^{i\omega_p t} + e^{-i\omega_p t}\right) + \mathcal{E}_c \frac{1}{2}\left(e^{i\omega_c t} + e^{-i\omega_c t}\right)\right)\wp_{31}e^{-i(\omega_1-\omega_3)t} \tag{12.2.11b}$$

$$(UH_IU^\dagger)_{23} = -\left(\boldsymbol{\mathcal{E}}_p \frac{1}{2}\left(e^{i\omega_p t} + e^{-i\omega_p t}\right) + \mathcal{E}_c \frac{1}{2}\left(e^{i\omega_c t} + e^{-i\omega_c t}\right)\right)\wp_{23}e^{i(\omega_2-\omega_3)t} \tag{12.2.11c}$$

$$(UH_1U^\dagger)_{32} = -\left(\boldsymbol{\mathcal{E}}_p \frac{1}{2}\left(e^{i\omega_p t} + e^{-i\omega_p t}\right) + \mathcal{E}_c \frac{1}{2}\left(e^{i\omega_c t} + e^{-i\omega_c t}\right)\right)\wp_{32}e^{-i(\omega_2-\omega_3)t} \tag{12.2.11d}$$

Afterwards, applying the Rotating Wave Approximation (RWA) (where terms containing the sums $\omega_3 - \omega_1 + \omega_p$ and $\omega_3 - \omega_2 + \omega_c$ are dropped)

$$(UH_IU^\dagger)_{13} = -\frac{1}{2}\boldsymbol{\mathcal{E}}_p\wp_{13}e^{i\left(\omega_1-\omega_{3+\omega_p}\right)t} \tag{12.2.12a}$$

$$(UH_IU^\dagger)_{31} = -\frac{1}{2}\boldsymbol{\mathcal{E}}_p\wp_{31}e^{-i\left(\omega_1-\omega_{3+\omega_p}\right)t} \tag{12.2.12b}$$

$$(UH_IU^\dagger)_{23} = -\frac{1}{2}\boldsymbol{\mathcal{E}}_c\wp_{23}e^{i(\omega_2-\omega_{3+\omega_c})t} \tag{12.2.12c}$$

$$(UH_1U^\dagger)_{32} = -\frac{1}{2}\boldsymbol{\mathcal{E}}_c\wp_{23}e^{-i(\omega_2-\omega_{3+\omega_c})t} \tag{12.2.12d}$$

Returning now to the Schrödinger picture by reversing the transformation as $U^\dagger(UH_IU^\dagger)U$ as follows

$$H_I = -\frac{\hbar}{2}\begin{pmatrix} 0 & 0 & \wp_{13}\boldsymbol{\mathcal{E}_p}e^{i\omega_p t} \\ 0 & 0 & \wp_{23}\boldsymbol{\mathcal{E}_c}e^{i\omega_c t} \\ \wp_{31}\boldsymbol{\mathcal{E}_p}e^{-i\omega_p t} & \wp_{32}\boldsymbol{\mathcal{E}_c}e^{-i\omega_c t} & 0 \end{pmatrix} \tag{12.2.13}$$

The dipole operator can be separated into magnitude and phase as

$$\wp_{13} = \wp_{31}^* = |\wp_{13}|e^{i\phi_p} \tag{12.2.14a}$$

$$\wp_{23} = \wp_{32}^{*} = |\wp_{23}|e^{i\phi_c}. \tag{12.2.14b}$$

Defining the Rabi frequencies as

$$\Omega_p = \frac{\mathcal{E}_p|\wp_1 3|}{\hbar} \tag{12.2.15a}$$

$$\Omega_c = \frac{\mathcal{E}_c|\wp_2 3|}{\hbar} \tag{12.2.15b}$$

we acquire the following result for H_I

$$H_I = -\frac{\hbar}{2}\begin{pmatrix} 0 & 0 & \Omega_p e^{i\phi_p}e^{i\omega_p t} \\ 0 & 0 & \Omega_c e^{i\phi_c}e^{i\omega_c t} \\ \Omega_p e^{-i\phi_p}e^{-i\omega_p t} & \Omega_c e^{-i\phi_c}e^{-i\omega_c t} & 0. \end{pmatrix} \tag{12.2.16}$$

From the combination of H_0 and H_I, we have the complete EIT Hamiltonian

$$H_{EIT} = \frac{\hbar}{2}\begin{pmatrix} 2\omega_1 & 0 & -\Omega_p e^{i\phi_p}e^{i\omega_p t} \\ 0 & 2\omega_2 & -\Omega_c e^{i\phi_c}e^{i\omega_c t} \\ -\Omega_p e^{-i\phi_p}e^{-i\omega_p t} & -\Omega_c e^{-i\phi_c}e^{-i\omega_c t} & 2\omega_3 \end{pmatrix} \tag{12.2.17}$$

Subsequently, another transformation is applied in order to remove all the time dependence from the Hamiltonian, as well as the phase of the dipole moment operator. The new basis is known as the rotating basis, which will be denoted with ˜'s on transformed elements. The new basis is related to the old one by $|\tilde{n}\rangle = \tilde{U}(t)\,|n\rangle$, where $\tilde{U}$ is given by

$$\tilde{U}(t) = \begin{pmatrix} e^{i\omega_p t}e^{i\phi_p} & 0 & 0 \\ 0 & e^{i\omega_c t}e^{i\phi_c} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{12.2.18}$$

For this transformation to be sensible, it must be unitary ($\tilde{U}(t)U(t) = \mathbb{I}$). Also the transformed Hamiltonian satisfies the Schrödinger equation,

$$\begin{aligned} \tilde{H}_{EIT}\,|\tilde{n}\rangle &= i\hbar\frac{\partial}{\partial t}\,|\tilde{n}\rangle \\ &= i\hbar\frac{\partial}{\partial t}\left(\tilde{U}\,|n\rangle\right) \\ &= i\hbar\left(\frac{\partial\tilde{U}}{\partial t}\tilde{n} + \tilde{U}\frac{\partial\,|n\rangle}{\partial t}\right) \\ &= i\hbar\left(\frac{\partial\tilde{U}}{\partial t}\tilde{n} + \frac{-i}{\hbar}\tilde{U}H_{EIT}\,|n\rangle\right) \\ &= \left(i\hbar\frac{\partial\tilde{U}}{\partial t}\tilde{U}^{\dagger} + \tilde{U}H_{EIT}\tilde{U}^{\dagger}\right)\tilde{U}\,|n\rangle\,\tilde{H}_{EIT}\,|\tilde{n}\rangle \\ &= \left(i\hbar\frac{\partial\tilde{U}}{\partial t}\tilde{U}^{d\dagger} + \tilde{U}H_{EIT}\tilde{U}^{\dagger}\right)|\tilde{n}\rangle \end{aligned} \tag{12.2.19}$$

The use of this transformation simplifies the Hamiltonian,

$$\begin{aligned}\tilde{H}_{EIT} &= i\hbar\frac{\partial\tilde{U}}{\partial t}\tilde{U}^{d\dagger} + \tilde{U}H_{EIT}\tilde{U}^{\dagger} \\ &= \frac{\hbar}{2}\begin{pmatrix}2\omega_p & 0 & 0\\ 0 & 2\omega_c & 0\\ 0 & 0 & 0\end{pmatrix} + \frac{\hbar}{2}\begin{pmatrix}2\omega_1 & 0 & -\Omega_p\\ 0 & 2\omega_2 & -\Omega_c\\ -\Omega_p & -\Omega_c & 2\omega_3\end{pmatrix} \\ \tilde{H}_{EIT} &= \frac{\hbar}{2}\begin{pmatrix}2(\omega_1+\omega_p) & 0 & -\Omega_p\\ 0 & 2(\omega_2+\omega_c) & -\Omega_c\\ -\Omega_p & -\Omega_c & 2\omega_3\end{pmatrix}\end{aligned} \tag{12.2.20}$$

The above Hamiltonian can be brought into its standard form by noting that we can add a multiple of the identity to the Hamiltonian without changing any physical results. Adding $-2(\omega_1 + \omega_p)\mathcal{I}$ to the Hamiltonian, Eq. 12.2.20 gives

$$\tilde{H}_{EIT} = \frac{\hbar}{2}\begin{pmatrix}0 & 0 & -\Omega_p\\ 0 & 2(\omega_2+\omega_c-\omega_1-\omega_p) & -\Omega_c\\ -\Omega_p & -\Omega_c & 2(\omega_3-\omega_1-\omega_p)\end{pmatrix} \tag{12.2.21}$$

Defining the laser detunings as

$$\Delta_p = \omega_p - \omega_3 + \omega_1 \tag{12.2.22a}$$

$$\Delta_c = \omega_c - \omega_3 + \omega_2 \tag{12.2.22b}$$

we obtain the following expression

$$\tilde{H}_{EIT} = \frac{\hbar}{2}\begin{pmatrix}0 & 0 & -\Omega_p\\ 0 & -2(\Delta_p-\Delta_c) & -\Omega_c\\ -\Omega_p & -\Omega_c & -2\Delta_p\end{pmatrix}. \tag{12.2.23}$$

12.3 Von - Neumann Master Equation

The EIT Hamiltonian, describes a single atom interacting with the external electromagnetic field, but in our system we have an ensemble of atoms. It is therefore natural to transition from describing the system with single atom wave functions, to describe it with density operators (ρ), which model the state of a population of atoms. Using the Von-Neumann equation, which is equivalent to the Schrödinger equation but has the benefit that it makes no reference to pure states,

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] \tag{12.3.1}$$

and taking into account effects which removes population from a given state, by adding in phenomenological decay terms

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{2}\{\Gamma, \rho\} \tag{12.3.2}$$

where Γ is defined by

$$\mathbf{\Gamma} = \begin{bmatrix}\Gamma_1 & 0 & 0\\ 0 & \Gamma_2 & 0\\ 0 & 0 & \Gamma_3\end{bmatrix}. \tag{12.3.3}$$

These added terms account for decays from each state for a general set of energy levels, but in a Λ system matters simplify. Firstly, Γ_1 will drop to zero, since conservation of energy prevents relaxations out of the ground state. Secondly, since $|2\rangle$ is a metastable state, Γ_2 will be dramatically smaller than Γ_3 ($\Gamma_2 << \Gamma_3$). The long lifetime of $|2\rangle$ is essential for maintaining coherence and EIT. The Von-Neumann Equation in component form is

$$\dot{\rho_{ij}} = \sum_k \left[-\frac{i}{\hbar}(H_{ik}\rho_{kj} - \rho_{ik}H_{kj}) - \frac{1}{2}(\Gamma_{ik}\rho_{kj} - \rho_{ik}\Gamma_{kj}) \right]. \tag{12.3.4}$$

We saw before that the Schrödinger equation holds in the new basis, and so, as they are equivalent, the Von-Neumann Equation also holds for $\tilde{\rho}$ and $\tilde{H}_{EIT}$.The resulting equations are:

$$\dot{\tilde{\rho}}_{11} = i\frac{\Omega_p}{2}(\tilde{\rho}_{31} - \tilde{\rho}_{13}) - \Gamma_1\tilde{\rho}_{11} \tag{12.3.5a}$$

$$\dot{\tilde{\rho}}_{22} = i\frac{\Omega_c}{2}(\tilde{\rho}_{32} - \tilde{\rho}_{23}) - \Gamma_2\tilde{\rho}_{22} \tag{12.3.5b}$$

$$\dot{\tilde{\rho}}_{33} = i\frac{1}{2}\left(\Omega_p(\tilde{\rho}_{13} - \tilde{\rho}_{31}) + \Omega_c(\tilde{\rho}_{23} - \tilde{\rho}_{32})\right) - \Gamma_3\tilde{\rho}_{33} \tag{12.3.5c}$$

$$\dot{\tilde{\rho}}_{12} = \dot{\tilde{\rho}}^*_{21} = i\frac{1}{2}\left[\Omega_p\tilde{\rho}_{32} - \Omega_c\tilde{\rho}_{13} + 2(\Delta_c - \Delta_p)\tilde{\rho}_{12}\right] - \frac{1}{2}(\Gamma_1 + \Gamma_2)\tilde{\rho}_{12} \tag{12.3.5d}$$

$$\dot{\tilde{\rho}}_{13} = \dot{\tilde{\rho}}^*_{31} = i\frac{1}{2}\left[\Omega_p(\tilde{\rho}_{33} - \tilde{\rho}_{11}) - \Omega_c\tilde{\rho}_{12} - 2\Delta_p\tilde{\rho}_{13}\right] - \frac{1}{2}(\Gamma_1 + \Gamma_3)\tilde{\rho}_{13} \tag{12.3.5e}$$

$$\dot{\tilde{\rho}}_{23} = \dot{\tilde{\rho}}^*_{32} = i\frac{1}{2}\left[-\Omega_p\tilde{\rho}_{21} + \Omega_c(\tilde{\rho}_{33} - \tilde{\rho}_{22}) - 2\Delta_c\tilde{\rho}_{23}\right] - \frac{1}{2}(\Gamma_2 + \Gamma_3)\tilde{\rho}_{23} \tag{12.3.5f}$$

where $*$'s represents complex conjugates. It is important to note that the Γ decay terms remove atoms from our population entirely. This aspect is undesired, since decays from $|2\rangle$ and $|3\rangle$ would not actually leave the system, but would instead decay to $|1\rangle$. We can fix this issue by noting that our system is being pumped into $|1\rangle$ by the action of the strong control beam. As long as our probe beam is weak, the atoms will primarily inhabit the $|1\rangle$ state in steady state solutions. This strong control beam assumption makes our system essentially conservative, allowing us to interpret the diagonal elements ρ_{ii} as the fraction of atoms in our ensemble that are in state $|i\rangle$. We can use the assumption of a strong control beam to simplify these equations. As we mentioned, the atoms will primarily be in the ground state $|1\rangle$, with few atoms in the excited states. This allows us to write

$$\tilde{\rho}_{11} \approx 1, \quad \tilde{\rho}_{22} \approx 0, \quad \tilde{\rho}_{33} \approx 0 \tag{12.3.6}$$

Substituting this approximation, it gives for the non-diagonal terms:

$$\dot{\tilde{\rho}}_{12,ss} = \dot{\tilde{\rho}}^*_{21,ss} = i\frac{1}{2}\left[\Omega_p\tilde{\rho}_{32} - \Omega_c\tilde{\rho}_{13} + 2(\Delta_c - \Delta_p)\tilde{\rho}_{12}\right] - \frac{1}{2}(\Gamma_1 + \Gamma_2)\tilde{\rho}_{12} \tag{12.3.7a}$$

$$\dot{\tilde{\rho}}_{13,ss} = \dot{\tilde{\rho}}^*_{31,ss} = i\frac{1}{2}\left[-\Omega_p - \Omega_c\tilde{\rho}_{12} - 2\Delta_p\tilde{\rho}_{13}\right] - \frac{1}{2}(\Gamma_1 + \Gamma_3)\tilde{\rho}_{13} \tag{12.3.7b}$$

$$\dot{\tilde{\rho}}_{23,ss} = \dot{\tilde{\rho}}^*_{32,ss} = i\frac{1}{2}\left[-\Omega_p\tilde{\rho}_{21} - 2\Delta_c\tilde{\rho}_{23}\right] - \frac{1}{2}(\Gamma_2 + \Gamma_3)\tilde{\rho}_{23} \tag{12.3.7c}$$

We search for the steady state solutions of $\tilde{\rho}_{12}$, $\tilde{\rho}_{13}$ and $\tilde{\rho}_{32}$. From the last set of equations, in steady state (where the derivative in respect to time t is zero) we obtain the solution for $\tilde{\rho}_{32}$

$$\tilde{\rho}_{32} = \frac{i\Omega_p\tilde{\rho}^{VN}_{12,ss}}{-i2\Delta_c + (\Gamma_2 + \Gamma_3)} \tag{12.3.8}$$

At this point, we can write the above system of equations for the off-diagonal terms $\tilde{\rho}_{12}$ and $\tilde{\rho}_{13}$ in matrix form as:

$$\dot{\boldsymbol{X}} = \boldsymbol{M} \cdot \boldsymbol{X} + \boldsymbol{A} \tag{12.3.9}$$

where

$$\boldsymbol{X} = \begin{bmatrix} \tilde{\rho}_{12} \\ \tilde{\rho}_{13} \end{bmatrix} \tag{12.3.10}$$

$$\boldsymbol{M}^{VN} = \begin{bmatrix} i\left(\Delta_c - \Delta_p\right) - \dfrac{1}{2}(\Gamma_1 + \Gamma_2) + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \frac{1}{2}(\Gamma_2 + \Gamma_3)} & -i\frac{1}{2}\Omega_c \\ -i\frac{1}{2}\Omega_c & -i\Delta_p - \frac{1}{2}(\Gamma_1 + \Gamma_3) \end{bmatrix} \tag{12.3.11}$$

and

$$\boldsymbol{A} = \begin{bmatrix} 0 \\ -i\frac{\Omega_p}{2} \end{bmatrix} \tag{12.3.12}$$

.

In steady state, where $\dot{\boldsymbol{X}} = 0$, the solution of the system is

$$\boldsymbol{X} = -\boldsymbol{M}^{-1}\boldsymbol{A}, \tag{12.3.13}$$

from where we obtain the following steady-state solutions:

$$\tilde{\rho}_{12,ss} = \frac{-\frac{1}{4}\Omega_c\Omega_p}{\left[i\left(\Delta_c - \Delta_p\right) - \dfrac{1}{2}(\Gamma_1 + \Gamma_2) + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \frac{1}{2}(\Gamma_2 + \Gamma_3)}\right]\left[-i\Delta_p - \frac{1}{2}(\Gamma_1 + \Gamma_3)\right] + \frac{1}{4}\Omega_c^2} \tag{12.3.14a}$$

$$\tilde{\rho}_{13,ss} = \frac{\left[i\left(\Delta_c - \Delta_p\right) - \dfrac{1}{2}(\Gamma_1 + \Gamma_2) + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \frac{1}{2}(\Gamma_2 + \Gamma_3)}\right]\left(i\frac{\Omega_p}{2}\right)}{\left[i\left(\Delta_c - \Delta_p\right) - \dfrac{1}{2}(\Gamma_1 + \Gamma_2) + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \frac{1}{2}(\Gamma_2 + \Gamma_3)}\right]\left[-i\Delta_p - \frac{1}{2}(\Gamma_1 + \Gamma_3)\right] + \frac{1}{4}\Omega_c^2} \tag{12.3.14b}$$

Overall, the steady solutions for the off-diagonal density matrix elements are the following:

$$\tilde{\rho}_{12,ss} = \tilde{\rho}_{21,ss}^{*} = \frac{-\frac{1}{4}\Omega_c\Omega_p}{\left[i\left(\Delta_c - \Delta_p\right) - \Gamma_{12} + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \Gamma_{23}}\right]\left[-i\Delta_p - \Gamma_{13}\right] + \frac{1}{4}\Omega_c^2} \tag{12.3.15a}$$

$$\tilde{\rho}_{13,ss} = \tilde{\rho}_{31,ss}^{*} = \frac{\left[i\left(\Delta_c - \Delta_p\right) - \Gamma_{12} + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \Gamma_{23}}\right]\left(i\frac{\Omega_p}{2}\right)}{\left[i\left(\Delta_c - \Delta_p\right) - \Gamma_{12} + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \Gamma_{23}}\right]\left[-i\Delta_p - \Gamma_{13}\right] + \frac{1}{4}\Omega_c^2} \tag{12.3.15b}$$

$$\tilde{\rho}_{32,ss} = \tilde{\rho}_{23,ss}^{*} = \frac{i\Omega_p\tilde{\rho}_{12,ss}}{2\left(-i\Delta_c + \Gamma_{23}\right)} \tag{12.3.15c}$$

where we defined as $\Gamma_{ij} = \frac{1}{2}\left(\Gamma_i + \Gamma_j\right)$ $(i, j = 1, 2, 3)$. Now, we have to go from density to susceptibility. We will see that the ρ_{13} element of the density matrix determines the susceptibility of the medium as seen by the probe. From this description of the medium, we can generate an expression of the macroscopic polarization in terms of the expectation of the dipole moment operators

$$\begin{aligned}\boldsymbol{P} &= N\left\langle \wp \right\rangle \\ &= NTr(\rho\wp) \\ &= N\left(\wp_{31}\rho_{13} + \wp_{32}\rho_{23} + \wp_{13}\rho_{31} + \wp_{23}\rho_{32}\right)\end{aligned} \tag{12.3.16}$$

where N is the density of atoms. We computed the density matrix elements in Eqs 12.3.15 in the rotating basis. We can convert these elements in the regular basis by using the inverse transformation $\rho = \tilde{U}^\dagger\tilde{\rho}\tilde{U}$

$$\rho = \tilde{U}^\dagger\tilde{\rho}\tilde{U} = \begin{bmatrix} \tilde{\rho}_{11} & \tilde{\rho}_{12}e^{i(\omega_p-\omega_c)t}e^{-i\phi_c}e^{i\phi_p} & \tilde{\rho}_{13}e^{i\omega_p t}e^{\phi_p} \\ \tilde{\rho}_{21}e^{-i(\omega_p-\omega_c)t}e^{i\phi_c}e^{-i\phi_p} & \tilde{\rho}_{22} & \tilde{\rho}_{23}e^{i\omega_c}e^{i\phi_c} \\ \tilde{\rho}_{31}e^{-i\omega_p t}e^{-\phi_p} & \tilde{\rho}_{32}e^{-i\omega_c}e^{-i\phi_c} & \tilde{\rho}_{33} \end{bmatrix} \tag{12.3.17}$$

or we can compute the inverse

$$\tilde{\rho} = \tilde{U}\rho\tilde{U}^\dagger = \begin{bmatrix} \rho_{11} & \rho_{12}e^{i(\omega_p-\omega_c)t}e^{-i\phi_c}e^{i\phi_p} & \rho_{13}e^{i\omega_p t}e^{\phi_p} \\ \rho_{21}e^{-i(\omega_p-\omega_c)t}e^{i\phi_c}e^{-i\phi_p} & \rho_{22} & \rho_{23}e^{i\omega_c}e^{i\phi_c} \\ \rho_{31}e^{-i\omega_p t}e^{-\phi_p} & \rho_{32}e^{-i\omega_c}e^{-i\phi_c} & \rho_{33} \end{bmatrix} \tag{12.3.18}$$

We can now write the polarization from Eq. 12.3.16 in terms of the known $\tilde{\rho}$ density matrix elements

$$\boldsymbol{P} = N\left(\wp_{31}\tilde{\rho}_{13}e^{i\omega_p t}e^{i\phi_p} + \wp_{32}\tilde{\rho}_{23}e^{i\omega_c t}e^{i\phi_c} + \wp_{13}\tilde{\rho}_{31}e^{-i\omega_p t}e^{-i\phi_p} + \wp_{23}\tilde{\rho}_{32}e^{-i\omega_c t}e^{-i\phi_c}\right), \tag{12.3.19}$$

Remembering that we are looking for the linear susceptibility χ, given by the $\boldsymbol{P} = \epsilon_0\chi\boldsymbol{E}$ and writing the electric field in full we have

$$\begin{aligned}\boldsymbol{P} &= \epsilon_0\chi\boldsymbol{E} \\ &= \chi\omega_p\epsilon_0\boldsymbol{\mathcal{E}}_p\frac{1}{2}\left(e^{i\omega_p t} + e^{-i\omega_p t}\right) + \chi\omega_c\epsilon_0\boldsymbol{\mathcal{E}}_c\frac{1}{2}\left(e^{i\omega_c t} + e^{-i\omega_c t}\right)\end{aligned} \tag{12.3.20}$$

Also, we have the relation

$$N\left\langle \wp \right\rangle = \epsilon_0\chi\boldsymbol{E}, \tag{12.3.21}$$

from which we can solve for χ. Using Eq. 12.3.21, comparing the last two equations, Eqs 12.3.19 and 12.3.20, from which we can match the time - dependent exponentials for ρ_{13}, and solving for $\chi(\omega_p)$ we get

$$\begin{aligned}\chi(\omega_p) &= \frac{2N\wp_{31}}{\epsilon_0\boldsymbol{\mathcal{E}}_p}\tilde{\rho}_{13}e^{i\phi_p} \\ &= \frac{2N|\wp_{13}|}{\epsilon_0\boldsymbol{\mathcal{E}}_p}\tilde{\rho}_{13}\end{aligned} \tag{12.3.22}$$

where Eq. 12.2.14a was used. Adding the solution for $\tilde{\rho}_{13}$ from Eq. 12.3.15b, the final equation for the susceptibility is

$$\chi(\omega_p) = \frac{2N|\wp_{13}|}{\epsilon_0\boldsymbol{\mathcal{E}}_p}\frac{\left[i\left(\Delta_c - \Delta_p\right) - \Gamma_{12} + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \Gamma_{23}}\right]\left(i\frac{\Omega_p}{2}\right)}{\left[i\left(\Delta_c - \Delta_p\right) - \Gamma_{12} + \dfrac{1}{4}\dfrac{\Omega_p^2}{i\Delta_c - \Gamma_{23}}\right]\left[-i\Delta_p - \Gamma_{13}\right] + \frac{1}{4}\Omega_c^2} \tag{12.3.23}$$

We now will split χ into real and imaginary components. After simplification, these are

$$\operatorname{Re}\left[\chi(\omega_p)\right] = \frac{2N|\wp_{13}|}{\epsilon_0 \boldsymbol{\mathcal{E}}_p} \frac{\Omega_p \left[\begin{array}{l} -\,\Omega_p^4\Delta_p \\ +\,\Omega_p^2\left(8\Delta_p(\Delta_c^2 - \Gamma_{12}\Gamma_{23}) - \Delta_c\left(8\Delta_p^2 - \Omega_c^2\right)\right) \\ -\,4(\Gamma_{23}^2 + \Delta_c^2)\left(4\Delta_p\left((\Delta_c - \Delta_p)^2 + \Gamma_{12}^2\right) + (\Delta_c - \Delta_p)\Omega_c^2\right) \end{array}\right]}{\left[\begin{array}{l} 2\Omega_p^4(\Gamma_{13}^2 + \Delta_p^2) \\ -\,4\Omega_p^2\left[\left(\Delta_c\Delta_p - \Gamma_{13}\Gamma_{23}\right)\Omega_c^2 + \left(\Delta_p^2 + \Gamma_{13}^2\right)\left(\Delta_c\left(4\Delta_c - \Delta_p - \Gamma_{12}\Gamma_{23}\right)\right)\right] \\ +\,2\left(\Gamma_{23}^2 + \Delta_c^2\right)\left[\begin{array}{l} \Omega_c^4 + 8\left(\Gamma_{12}\Gamma_{13} + \Delta_p(\Delta_c - \Delta_p)\right)\Omega_c^2 \\ +\,16\left(\Delta_p^2 + \Gamma_{13}^2\right)\left((\Delta_c - \Delta_p)^2 + \Gamma_{12}^2\right) \end{array}\right] \end{array}\right]} \tag{12.3.24a}$$

$$\operatorname{Im}\left[\chi(\omega_p)\right] = \frac{2N|\wp_{13}|}{\epsilon_0 \boldsymbol{\mathcal{E}}_p} \frac{\Omega_p \left[\begin{array}{l} -\,\Omega_p^4\Gamma_{13} \\ +\,\Omega_p^2\left(8\Gamma_{13}\left(\Delta_c\left(\Delta_c - \Delta_p\right) - \Gamma_{12}\Gamma_{13}\right) - \Gamma_{23}\Omega_c^2\right) \\ -\,4\left(\Gamma_{23}^2 + \Delta_c^2\right)\left[4\Gamma_{13}\left((\Delta_c - \Delta_p)^2 + \Gamma_{12}^2\right) + \Gamma_{12}\Omega_c^2\right] \end{array}\right]}{\left[\begin{array}{l} 2\Omega_p^4(\Gamma_{13}^2 + \Delta_p^2) \\ -\,4\Omega_p^2\left[\left(\Delta_c\Delta_p - \Gamma_{13}\Gamma_{23}\right)\Omega_c^2 + \left(\Delta_p^2 + \Gamma_{13}^2\right)\left(\Delta_c\left(4\Delta_c - \Delta_p - \Gamma_{12}\Gamma_{23}\right)\right)\right] \\ +\,2\left(\Gamma_{23}^2 + \Delta_c^2\right)\left[\begin{array}{l} \Omega_c^4 + 8\left(\Gamma_{12}\Gamma_{13} + \Delta_p(\Delta_c - \Delta_p)\right)\Omega_c^2 \\ +\,16\left(\Delta_p^2 + \Gamma_{13}^2\right)\left((\Delta_c - \Delta_p)^2 + \Gamma_{12}^2\right) \end{array}\right] \end{array}\right]} \tag{12.3.24b}$$

12.4 Lindblad Master Equation

In this section we will apply the Lindblad master equation, in order to study the phenomenon of the electromagnetically induced transparency (EIT). We will in the basis of $|n\rangle$ and the Hamiltonian that describe our system of interest will be the respective one that we saw earlier, after the application of the rotating wave approximation (RWA). So the EIT Hamiltonian in this case is of the form:

$$\begin{aligned}
H_{EIT} &= \frac{\hbar}{2}\begin{bmatrix} 2\omega_1 & 0 & -\Omega_p e^{i\omega_p t}e^{i\phi_p} \\ 0 & 2\omega_2 & -\Omega_c e^{i\omega_c t}e^{i\phi_c} \\ -\Omega_p e^{-i\omega_p t}e^{-i\phi_p} & -\Omega_c e^{-i\omega_c t}e^{-i\phi_c} & 2\omega_3 \end{bmatrix} = \\
&= \hbar\begin{bmatrix} \omega_1 & 0 & -\frac{\Omega_p}{2} e^{i\omega_p t}e^{i\phi_p} \\ 0 & \omega_2 & -\frac{\Omega_c}{2} e^{i\omega_c t}e^{i\phi_c} \\ -\frac{\Omega_p}{2} e^{-i\omega_p t}e^{-i\phi_p} & -\frac{\Omega_c}{2} e^{-i\omega_c t}e^{-i\phi_c} & \omega_3 \end{bmatrix} \overset{-\omega_1\mathbb{I}}{=} \\
&= \hbar\begin{bmatrix} 0 & 0 & -\frac{\Omega_p}{2} e^{i\omega_p t}e^{i\phi_p} \\ 0 & \omega_2-\omega_1 & -\frac{\Omega_c}{2} e^{i\omega_c t}e^{i\phi_c} \\ -\frac{\Omega_p}{2} e^{-i\omega_p t}e^{-i\phi_p} & -\frac{\Omega_c}{2} e^{-i\omega_c t}e^{-i\phi_c} & \omega_3-\omega_1 \end{bmatrix} = \\
&= \hbar\begin{bmatrix} 0 & 0 & -\frac{\Omega_p}{2} e^{i\omega_p t}e^{i\phi_p} \\ 0 & (\omega_3-\omega_1)-(\omega_3-\omega_2) & -\frac{\Omega_c}{2} e^{i\omega_c t}e^{i\phi_c} \\ -\frac{\Omega_p}{2} e^{-i\omega_p t}e^{-i\phi_p} & -\frac{\Omega_c}{2} e^{-i\omega_c t}e^{-i\phi_c} & \omega_3-\omega_1 \end{bmatrix} \overset{\left\{\begin{smallmatrix} (\omega_3-\omega_1)=\omega_p\pm\Delta_p \\ (\omega_3-\omega_2)=\omega_c\pm\Delta_c \end{smallmatrix}\right\}}{=} \\
&= \hbar\begin{bmatrix} 0 & 0 & -\frac{\Omega_p}{2} e^{i\omega_p t}e^{i\phi_p} \\ 0 & \omega_p\pm\Delta_p-(\omega_c\pm\Delta_c) & -\frac{\Omega_c}{2} e^{i\omega_c t}e^{i\phi_c} \\ -\frac{\Omega_p}{2} e^{-i\omega_p t}e^{-i\phi_p} & -\frac{\Omega_c}{2} e^{-i\omega_c t}e^{-i\phi_c} & \omega_p\pm\Delta_p \end{bmatrix} \Rightarrow \\
H_{EIT} &= \hbar\begin{bmatrix} 0 & 0 & -\frac{\Omega_p}{2} e^{i\omega_p t}e^{i\phi_p} \\ 0 & (\omega_p\pm\Delta_p)-(\omega_c\pm\Delta_c) & -\frac{\Omega_c}{2} e^{i\omega_c t}e^{i\phi_c} \\ -\frac{\Omega_p}{2} e^{-i\omega_p t}e^{-i\phi_p} & -\frac{\Omega_c}{2} e^{-i\omega_c t}e^{-i\phi_c} & (\omega_p\pm\Delta_p) \end{bmatrix}
\end{aligned} \tag{12.4.1}$$

which has time and phase dependence.

The Lindblad master equation has the following expression [25]:

$$\begin{aligned}
\dot{\rho} = -i[H_{EIT},\rho] &+ \sum_{\omega\geq 0}\alpha(\omega)e^{\beta\omega}\left(L_\omega\rho L_\omega^\dagger - \frac{1}{2}\{L_\omega^\dagger L_\omega,\rho\}\right) \\
&+ \sum_{\omega>0}\alpha(\omega)\left(L_\omega^\dagger\rho L_\omega - \frac{1}{2}\{L_\omega L_\omega^\dagger,\rho\}\right) \\
&+ \sum_{\omega_{ii}}\alpha(0)\left(L_{\omega_{ii}}\rho L_{\omega_{ii}} - \frac{1}{2}\{L_{\omega_{ii}}L_{\omega_{ii}},\rho\}\right)
\end{aligned} \tag{12.4.2}$$

where $\omega = \{\omega_{12},\omega_{13},\omega_{23}\}$ is the set of the possible transitions, L_ω are the Lindblad operators, $\alpha(\omega)$ is a real quantity, responsible for the absorption processes which take place. We will refer to these terms analytically later on.

In order to find the steady-state solution for the ρ_{13} density matrix element, which as we saw in the previous section is proportional to the electric susceptibility $\chi(\omega_p)$, we have to integrate in respect to time the set of the differential equations. At this point, it is necessary to follow the steps below in order to apply this scheme:

- First, we have to diagonalize the Hamiltonian $\hat{H}_{EIT} = U^\dagger H_{EIT} U$ to get the N eigenvalues E_i but also the N eigenvectors $|E_i\rangle$ to construct the base change matrix U.

- Next, go to the basis of the $\hat{H}_{EIT}$, i.e. apply the transformation $Q = U^{\dagger}Q_0U$ to the coupling operator.

- Then, compute the set of eigenfrequencies $\omega_{ij} = E_i - E_j$ from the eigenvalues of the Hamiltonian $\hat{H}_{EIT}$.

- Eliminate possible duplicated frequencies ω_{ij} (originating from equally spaced energy levels produced by degeneracies in the Hamiltonian) to construct the set of eigenfrequencies ω.

- Use $\langle E_i \,|\, L_\omega \,|\, E_j \rangle = \langle E_i \,|\, Q \,|\, E_j \rangle \, \delta_{kr} \left(E_i - E_j, -\omega \right)$ to construct the matrix element of the different Lindblad operators:
  - Each time that a $(E_i - E_j)$ match with a given $-\omega$, we put the coefficient Q_{ij} at position (i, j) in the Lindblad operator L_ω (this procedure take into account degeneracies).

- The Lindblad operators L_ω are defined in the basis where the Hamitlonian is diagonal so that they are already in the right basis (no transformation needed).

- The absorption rate $\alpha(\omega)$ are then computed for the different unique frequencies ω obtained and the corresponding emission rate are given by the detailed balance $e(\omega) = e^{\beta\omega}\alpha(\omega)$:
  - For a bosonic bath, we for example, use $\alpha(|\omega|) = \frac{\gamma}{\beta}\frac{\beta|\omega|}{e^{|\beta|\omega}-1}$ so that at high temperature it converges to $\alpha(\omega) = \frac{\gamma}{\beta}$. Moreover, the case $\alpha(0) = \frac{\gamma}{\beta}$ is well defined.

- For a time-dependent Hamiltonian $H_{EIT}(t)$, this procedure has to be re-iterated at each time step of the simulation giving rise to a time-dependent detailed balance (the system converges at each time step to a different Gibbs state due to the time-dependence of the Hamiltonian). Hence, the matrix elements change in time producing time-dependent Lindblad operators $\langle E_i(t) \,|\, L_\omega \,|\, E_j(t) \rangle = \langle E_i(t) \,|\, Q \,|\, E_j(t) \rangle$ $\delta_{kr} \left(E_i(t) - E_j(t), -\omega \right)$ where ω comes from $\hat{H}_{EIT}(t)$. Absorption $\alpha(\omega)$ and emission $e(\omega)$ rates are recomputed at each time step too.

- As a final check, one could compute the two sides of $[L_\omega(t), \hat{H}_{EIT}(t)] = \omega L_\omega(t)$ for one or more $L_\omega(t)$ to check the procedure.

According to the procedure described above, $\omega_{ij} = \lambda_j - \lambda_i$ where λ_k $(k = 1, 2, 3)$ are the eigenvalues of H_{EIT}, in ascending order. The term $\alpha(\omega)$ is chosen to be of the form:

$$\alpha(\omega) = \frac{\gamma}{\beta}\frac{\beta\omega}{e^{\beta\omega} - 1} \tag{12.4.3}$$

with $\beta = \frac{1}{k_B T_e}$. In the case of the dephasing terms, $\alpha(0) = \frac{\gamma}{\beta}$. Also, the initial expression of the coupling operator Q

$$\boldsymbol{Q}_0 = \begin{bmatrix} 0 & 0 & Q_{0_{13}} \\ 0 & 0 & Q_{0_{23}} \\ Q^*_{0_{13}} & Q^*_{0_{23}} & 0 \end{bmatrix} \tag{12.4.4}$$

where we put the values of the elements (12) and (21) to zero as our three-level system is of Λ-configuration with the $|1\rangle \rightarrow |2\rangle$ being dipole-forbidden, Also, we neglect the diagonal terms, which does not affect the steady-state solution but the dynamics of the system [25]. The general form of the coupling operator, since we go to the energy basis through the transformation $\boldsymbol{Q} = \boldsymbol{U}^{\dagger}\boldsymbol{Q}_0\boldsymbol{U}$ is

$$\boldsymbol{Q} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{bmatrix} \tag{12.4.5}$$

where $\boldsymbol{U}$ is the base change matrix (to the Hamiltonian basis) including the corresponding eigenvectors (to the eigenvalues) of H_{EIT}. Then, we are in position to define the Lindblad operators, as shown below:

$$\boldsymbol{L}_{12} = \begin{bmatrix} 0 & Q_{12} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \boldsymbol{L}_{12}^{\dagger} = \begin{bmatrix} 0 & 0 & 0 \\ Q_{21} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{12.4.6a}$$

$$\boldsymbol{L}_{13} = \begin{bmatrix} 0 & 0 & Q_{13} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \boldsymbol{L}_{13}^{\dagger} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ Q_{31} & 0 & 0 \end{bmatrix} \tag{12.4.6b}$$

$$\boldsymbol{L}_{23} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & Q_{23} \\ 0 & 0 & 0 \end{bmatrix} \qquad \boldsymbol{L}_{23}^{\dagger} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & Q_{32} & 0 \end{bmatrix} \tag{12.4.6c}$$

$$\boldsymbol{L}_{11} = \boldsymbol{L}_{11}^{\dagger} = \begin{bmatrix} Q_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \boldsymbol{L}_{22} = \boldsymbol{L}_{22}^{\dagger} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & Q_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \boldsymbol{L}_{33} = \boldsymbol{L}_{33}^{\dagger} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & Q_{33} \end{bmatrix} \tag{12.4.6d}$$

The resulting equations for the density matrix acquired through the Lindblad master equation are:

$$\dot{\rho}_{11} = i\,\frac{1}{2}\,\Omega_p \left(\begin{array}{l} e^{i\omega_p t}e^{i\phi_p}\rho_{31} \\ -\,e^{-i\omega_p t}e^{-i\phi_p}\rho_{13} \end{array}\right) + \left[\begin{array}{l} \alpha(\omega_{12})\left(e^{\beta\omega_{12}}\rho_{22}-\rho_{11}\right)Q_{12}Q_{21} \\ +\,\alpha(\omega_{13})\left(e^{\beta\omega_{13}}\rho_{33}-\rho_{11}\right)Q_{13}Q_{31} \end{array}\right] \tag{12.4.7a}$$

$$\dot{\rho}_{22} = i\,\frac{1}{2}\,\Omega_c \left(\begin{array}{l} e^{i\omega_c t}e^{i\phi_c}\rho_{32} \\ -\,e^{-i\omega_c t}e^{-i\phi_c}\rho_{23} \end{array}\right) + \left[\begin{array}{l} -\,\alpha(\omega_{12})\left(e^{\beta\omega_{12}}\rho_{22}-\rho_{11}\right)Q_{12}Q_{21} \\ +\,\alpha(\omega_{23})\left(e^{\beta\omega_{23}}\rho_{33}-\rho_{22}\right)Q_{23}Q_{32} \end{array}\right] \tag{12.4.7b}$$

$$\dot{\rho}_{33} = i\frac{1}{2}\left[\begin{array}{l} \Omega_p\left(e^{-i\omega_p t}e^{-i\phi_p}\rho_{13}-e^{i\omega_p t}e^{i\phi_p}\rho_{31}\right) \\ +\,\Omega_c\left(e^{-i\omega_c t}e^{-i\phi_c}\rho_{23}-e^{i\omega_c t}e^{i\phi_c}\rho_{32}\right) \end{array}\right] + \left[\begin{array}{l} -\,\alpha(\omega_{13})Q_{13}Q_{31}\left(e^{\beta\omega_{13}}\rho_{33}-\rho_{11}\right) \\ -\,\alpha(\omega_{23})Q_{23}Q_{32}\left(e^{\beta\omega_{23}}\rho_{33}-\rho_{22}\right) \end{array}\right] \tag{12.4.7c}$$

$$\dot{\rho}_{12} = \dot{\rho}_{21}^{*} = i\,\frac{1}{2}\left[\begin{array}{l} \Omega_p e^{i\omega_p t}e^{i\phi_p}\rho_{32}-\Omega_c e^{-i\omega_c t}e^{-i\phi_c}\rho_{13} \\ +\,2\left(\omega_p-\left(\Delta_p-\omega_c\pm\Delta_c\right)\right)\rho_{12} \end{array}\right] - \frac{1}{2}\left[\begin{array}{l} \alpha(\omega_{12})Q_{12}Q_{21}(e^{\beta\omega_{12}}+1) \\ +\,\alpha(\omega_{13})Q_{13}Q_{31} \\ +\,\alpha(\omega_{23})Q_{23}Q_{32} \\ +\,\alpha(0)Q_{11}^2+\alpha(0)Q_{22}^2 \end{array}\right]\rho_{12} \tag{12.4.7d}$$

$$\dot{\rho}_{13} = \dot{\rho}_{31}^{*} = -i\,\frac{1}{2}\left[\begin{array}{l} \Omega_p e^{i\omega_p t}e^{i\phi_p}\left(\rho_{11}-\rho_{33}\right) \\ +\,\Omega_c e^{i\omega_c t}e^{i\phi_c}\rho_{12} \\ -\,2\left(\omega_p\pm\Delta_p\right)\rho_{13} \end{array}\right] - \frac{1}{2}\left[\begin{array}{l} \alpha(\omega_{12})Q_{12}Q_{21} \\ +\,\alpha(\omega_{13})Q_{13}Q_{31}\left(e^{\beta\omega_{13}}+1\right) \\ +\,\alpha(\omega_{23})Q_{23}Q_{32}e^{\beta\omega_{23}} \\ +\,\alpha(0)Q_{11}^2+\alpha(0)Q_{33}^2 \end{array}\right]\rho_{13} \tag{12.4.7e}$$

$$\dot{\rho}_{23} = \dot{\rho}_{32}^{*} = -i\,\frac{1}{2}\left[\begin{array}{l} \Omega_p e^{i\omega_p t}e^{i\phi_p}\rho_{21} \\ +\,\Omega_c e^{i\omega_c t}e^{i\phi_c}\left(\rho_{22}-\rho_{33}\right) \\ -\,\left(\omega_c\pm\Delta_c\right)\rho_{23} \end{array}\right] - \frac{1}{2}\left[\begin{array}{l} \alpha(\omega_{12})Q_{12}Q_{21}e^{\beta\omega_{12}} \\ +\,\alpha(\omega_{13})Q_{13}Q_{31}e^{\beta\omega_{13}} \\ +\,\alpha(\omega_{23})Q_{23}Q_{32}\left(e^{\beta\omega_{23}}+1\right) \\ +\,\alpha(0)Q_{22}^2+\alpha(0)Q_{33}^2 \end{array}\right]\rho_{23} \tag{12.4.7f}$$

Assuming that at steady state, mainly the ground state will be populated, we can write that: $\rho_{11} \approx 1$, $\rho_{22} \approx 0$, $\rho_{33} \approx 0$ and the simplified equations for the off-diagonal terms read:

$$\dot{\rho}_{12} = \dot{\rho}_{21}^{*} = i\,\frac{1}{2}\begin{bmatrix} \Omega_p e^{i\omega_p t} e^{i\phi_p} \rho_{32} \\ -\,\Omega_c e^{-i\omega_c t} e^{-i\phi_c} \rho_{13} \\ +\,2\begin{pmatrix} \omega_p \pm \Delta_p \\ -\,(\omega_c \pm \Delta_c) \end{pmatrix} \rho_{12} \end{bmatrix} - \frac{1}{2}\begin{bmatrix} \alpha(\omega_{12}) Q_{12} Q_{21} (e^{\beta\omega_{12}} + 1) \\ +\,\alpha(\omega_{13}) Q_{13} Q_{31} \\ +\,\alpha(\omega_{23}) Q_{23} Q_{32} \\ +\,\alpha(0) Q_{11}^2 + \alpha(0) Q_{22}^2 \end{bmatrix} \rho_{12} \tag{12.4.8a}$$

$$\dot{\rho}_{13} = \dot{\rho}_{31}^{*} = -i\,\frac{1}{2}\begin{bmatrix} \Omega_p e^{i\omega_p t} e^{i\phi_p} \\ +\,\Omega_c e^{i\omega_c t} e^{i\phi_c} \rho_{12} \\ -\,2\left(\omega_p \pm \Delta_p\right) \rho_{13} \end{bmatrix} - \frac{1}{2}\begin{bmatrix} \alpha(\omega_{12}) Q_{12} Q_{21} \\ +\,\alpha(\omega_{13}) Q_{13} Q_{31} \left(e^{\beta\omega_{13}} + 1\right) \\ +\,\alpha(\omega_{23}) Q_{23} Q_{32} e^{\beta\omega_{23}} \\ +\,\alpha(0) Q_{11}^2 + \alpha(0) Q_{33}^2 \end{bmatrix} \rho_{13} \tag{12.4.8b}$$

$$\dot{\rho}_{23} = \dot{\rho}_{32}^{*} = -i\,\frac{1}{2}\begin{bmatrix} \Omega_p e^{i\omega_p t} e^{i\phi_p} \rho_{21} \\ -\,2\left(\omega_c \pm \Delta_c\right) \rho_{23} \end{bmatrix} - \frac{1}{2}\begin{bmatrix} \alpha(\omega_{12}) Q_{12} Q_{21} e^{\beta\omega_{12}} \\ +\,\alpha(\omega_{13}) Q_{13} Q_{31} e^{\beta\omega_{13}} \\ +\,\alpha(\omega_{23}) Q_{23} Q_{32} \left(e^{\beta\omega_{23}} + 1\right) \\ +\,\alpha(0) Q_{22}^2 + \alpha(0) Q_{33}^2 \end{bmatrix} \rho_{23} \tag{12.4.8c}$$

Defining:

$$D_{12} = \frac{1}{2}\begin{bmatrix} \alpha(\omega_{12}) Q_{12} Q_{21} (e^{\beta\omega_{12}} + 1) \\ +\,\alpha(\omega_{13}) Q_{13} Q_{31} \\ +\,\alpha(\omega_{23}) Q_{23} Q_{32} \\ +\,\alpha(0) Q_{11}^2 + \alpha(0) Q_{22}^2 \end{bmatrix} \tag{12.4.9a}$$

$$D_{13} = \frac{1}{2}\begin{bmatrix} \alpha(\omega_{12}) Q_{12} Q_{21} \\ +\,\alpha(\omega_{13}) Q_{13} Q_{31} \left(e^{\beta\omega_{13}} + 1\right) \\ +\,\alpha(\omega_{23}) Q_{23} Q_{32} e^{\beta\omega_{23}} \\ +\,\alpha(0) Q_{11}^2 + \alpha(0) Q_{33}^2 \end{bmatrix} \tag{12.4.9b}$$

$$D_{23} = \frac{1}{2}\begin{bmatrix} \alpha(\omega_{12}) Q_{12} Q_{21} e^{\beta\omega_{12}} \\ +\,\alpha(\omega_{13}) Q_{13} Q_{31} e^{\beta\omega_{13}} \\ +\,\alpha(\omega_{23}) Q_{23} Q_{32} \left(e^{\beta\omega_{23}} + 1\right) \\ +\,\alpha(0) Q_{22}^2 + \alpha(0) Q_{33}^2 \end{bmatrix} \tag{12.4.9c}$$

we get

$$\dot{\rho}_{12} = \dot{\rho}_{21}^{*} = i\,\frac{1}{2}\left[\begin{array}{l} \Omega_p e^{i\omega_p t} e^{i\phi_p} \rho_{32} \\ -\,\Omega_c e^{-i\omega_c t} e^{-i\phi_c} \rho_{13} \\ +\,2\left(\omega_p \pm \Delta_p - (\omega_c \pm \Delta_c)\right) \rho_{12} \end{array}\right] - D_{12}\rho_{12} \tag{12.4.10a}$$

$$\dot{\rho}_{13} = \dot{\rho}_{31}^{*} = -i\,\frac{1}{2}\left[\begin{array}{l} \Omega_p e^{i\omega_p t} e^{i\phi_p} \\ +\,\Omega_c e^{i\omega_c t} e^{i\phi_c} \rho_{12} \\ -\,2\left(\omega_p \pm \Delta_p\right) \rho_{13} \end{array}\right] - D_{13}\rho_{13} \tag{12.4.10b}$$

$$\dot{\rho}_{23} = \dot{\rho}_{32}^{*} = -i\,\frac{1}{2}\left[\begin{array}{l} \Omega_p e^{i\omega_p t} e^{i\phi_p} \rho_{21} \\ -\,2\left(\omega_c \pm \Delta_c\right) \rho_{23} \end{array}\right] - \frac{1}{2} D_{23}\rho_{23} \tag{12.4.10c}$$

In order to extract the solutions of ρ_{ij}, we follow the steps below:

a. Perform time integration of the Lindblad master equation, Eqs 12.4.7, for a specific value of Δ_p.

b. In steady state, the solution of the non-diagonal terms (both real and imaginary parts) shows an oscillatory behaviour. For the specification of the susceptibility $\chi(\omega_p)$, we only need the element ρ_{13}. So, we fit its solution with a (wave) function of the form $\rho_{13} = A_{13} e^{i\omega_{13} t} e^{\phi_{13}}$, from where we obtain A_{13} and ϕ_{13} with $\omega_{13} \equiv \omega_p$ fixed.

c. Determine the susceptibility through the relation $\chi(\omega_p) = A_{13} e^{i\phi_{13}}$.

d. Repeat this procedure for several values of Δ_p.

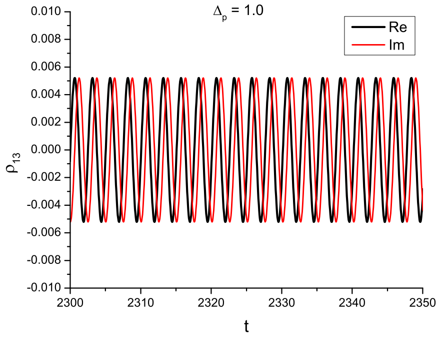


Figure 12.4.1: Typical example of the oscillatory behaviour of the solution of ρ_{13} density matrix element (real and imaginary part) obtained from the Lindblad master equation, for a specific value of Δ_p.

In the following section we present results obtained from both master equations, for the susceptibility of the system with respect to the probe field.

12.4.1 Results

In this section we present results referring to the susceptibility, χ, of the system with respect to the probe field, Δ_p, through two master equations.

The first one, a modified Von-Neumann master equation, is an empirical one allowing for decays from each energy state. In this case, an analytical solution is possible, Eqs 12.3.15, 12.3.23.

The other equation is a typical Lindblad one, with time-dependent operators from which only numerical results can be obtained. The procedure for the time integration of the corresponding equations, Eqs 12.4.7, is described in the previous section. Although the Lindblad operators should be updated in every time step, here they are computed once (at the beginning) and then are kept constant. However, we observe the EIT phenomenon. We can see below the referring results:

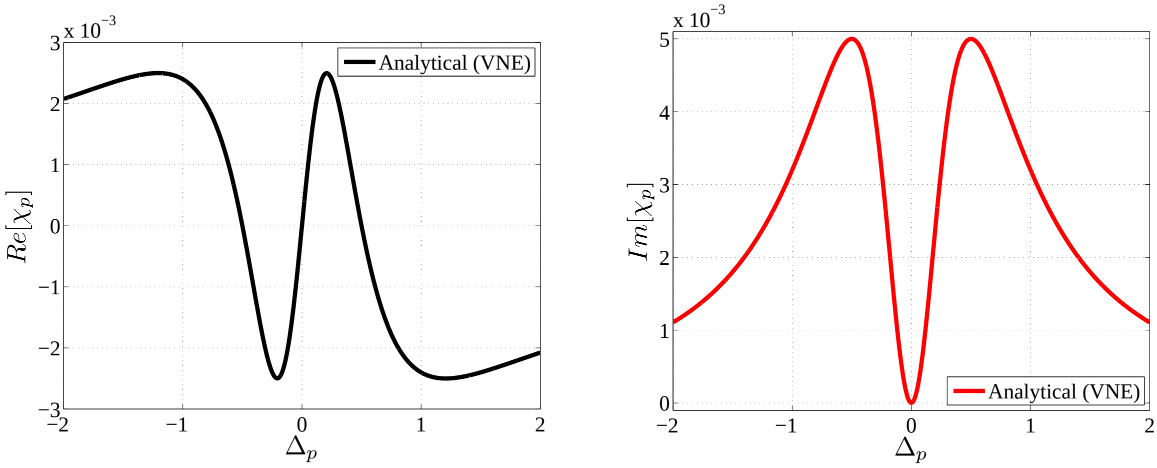


Figure 12.4.1: Analytical solution for the electric susceptibility (real and imaginary part) acquired through the Von-Neumann Master Equation (VNE).

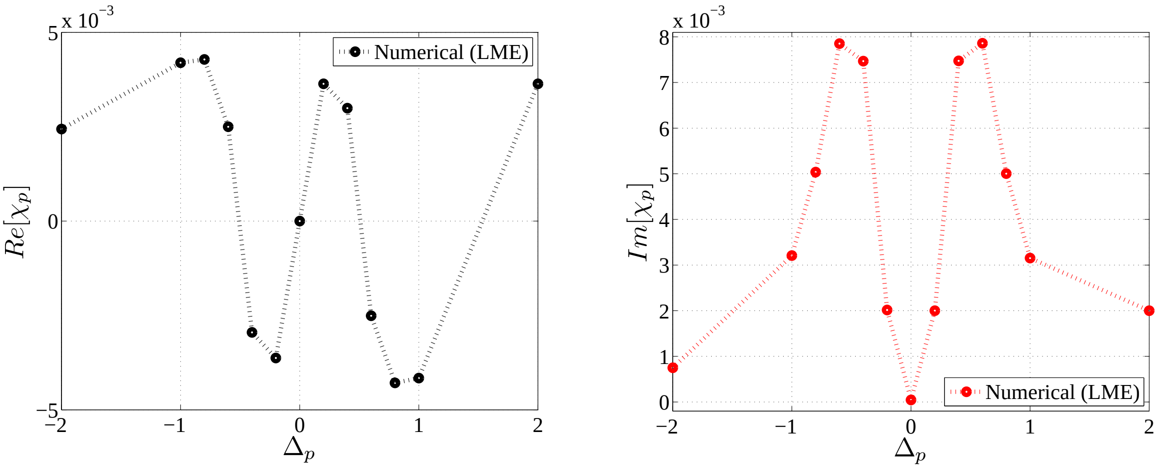


Figure 12.4.2: Numerical solution for the electric susceptibility (real and imaginary part) acquired through the Lindblad Master Equation (LME).

The input data for the exact results are the following:

$$
\begin{aligned}
&\Delta_c = 0, \quad \Omega_c = 1.2, \quad \Omega_p = \frac{1}{50}, \quad T_e = 0.2, \quad \gamma = 0.01, \\
&\boldsymbol{Q}_0 = \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 10i \\ -i & -10i & 0 \end{bmatrix}
\end{aligned}
\tag{12.4.1}
$$

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