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Relaxation in harmonic oscillator systems and wave propagation in negative index materials

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Relaxation in harmonic oscillator systems and wave propagation in negative index materials

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Dedicated to Shielonoi

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Relaxation in harmonic oscillator systems and wave propagation in negative index materials

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This dissertation is divided up into two parts, each examining a distinct theme. The first part of our work concerns itself with open quantum systems and the relaxation phenomena arising from the repeated application of an interaction Hamiltonian on systems composed of quantum harmonic oscillators. For the second part of our work, we shift gears and investigate the wave propagation in left-handed media, or materials with simultaneously negative electric permeability ϵ and magnetic permeability μ. Each of these two parts is complete within its own context.

In the first part of this dissertation, we introduce a relaxation-generating model which we use to study the process by which quantum correlations are created when an interaction Hamiltonian is repeatedly applied to bipartite harmonic oscillator systems for some characteristic time interval τ. The two important time scales which enter our results are discussed in detail. We show that the relaxation time obtained by the application of this repeated interaction scheme is proportional to both the strength of interaction and to the characteristic time interval τ. Through discussing the implications of our model, we show that, for the case where the oscillator frequencies are equal, the initial Maxwell-Boltzmann distributions of the uncoupled parts evolve to a new Maxwell-Boltzmann distribution through a series of transient Maxwell-Boltzmann distributions, or quasi-stationary, non-equilibrium states. We further analyze the case in which the two oscillator frequencies are unequal and show how the application of the same model leads to a non-thermal steady state. The calculations are exact and the results are obtained through an iterative process, without using perturbation theory.

In the second part of this dissertation, we examine the response of a plane wave incident on a flat surface of a left-handed material, a medium characterized by simultaneously negative electric permittivity ϵ and magnetic permeability μ. We do this by solving Maxwell's equations explicitly. In the literature up to date, it has been assumed that negative refractive materials are necessarily frequency dispersive. We propose an alternative to this assumption by suggesting that the requirement of positive energy density can be relaxed, and discuss the implications of such a proposal. More specifically, we show that once negative energy solutions are accepted, the requirement for frequency dispersion is no longer needed. We further argue that, for the purposes of discussing left-handed materials, the use of group velocity as the physically significant quantity is misleading, and suggest that any discussion involving it should be carefully reconsidered.

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Chapter 1

Introduction

1.1 Prologue

1.1.1 Relaxation in harmonic oscillator systems

Systems which do not suffer from unwanted interactions with the outside world are known as *closed* systems. However, in the real world, there are no perfectly closed systems, except perhaps the universe as a whole. Unwanted interactions with the outside world are inevitable. Systems in which the interaction with the environment is taken into consideration are known as *open* systems. For example, in quantum information processing, these interactions enter the problem in the form of noise. To be able to build useful information processing devices, the origin and behavior of such noises needs to be understood and controlled.

The interaction between two isolated systems can be a resource for quantum information processing [39]. However, the interaction between an isolated system and the environment surrounding it can lead to decoherence, an undesirable loss of information that was initially available. One way or the other, any interaction between two initially uncoupled subsystems leads to the exchange of quantities such as purity or polarization [55], or for thermodynamical systems, heat. To understand

and to control this interaction process, as well as to prevent decoherence, we need to study the mechanism by which this exchange occurs.

There has been a lot of interest and work in this problem [36, 53, 76, 78, 79, 82, 85]. Most of this work involves the coupling between two (or more) two-level quantum systems, or qubits, the fundamental units used in quantum computing [57, 58, 86, 89]. In this dissertation, we investigate the problem of interacting quantum systems which have larger state spaces. Specifically, we concentrate our attention to the study of the interaction between quantum systems with infinite-dimensional Hilbert spaces by considering the reduced dynamics of a harmonic oscillator induced by the evolution of a bipartite system which is also infinite-dimensional.

Any kind of optical or magnetic atomic trap can be modeled as a quantum harmonic oscillator (at least to the first order). Optical traps use laser beams to trap atoms, while magnetic traps use strong magnetic fields. Bose Einstein condensates can be created in either one of this kind of traps by forcing the atoms to fall to the ground state. Atomic traps are conservative in nature. In other words, energy is conserved and there is no friction. Any damping has to be added externally through some other means (just like friction in a mechanical oscillator). The analog of friction for trapped atoms can be created by forcing the atom to absorb a photon and spontaneously emit it. Measurements of the decoherence of a single trapped atom due to its coupling to engineered harmonic oscillator reservoirs with controllable states and controllable coupling are presented in [38]. Decoherence of specific quantum superpositions with a variety of couplings to a reservoir has been investigated extensively both theoretically and experimentally in [5, 6, 9, 51, 81], while sources of decoherence in the context of trapped-ion experiments have been more recently discussed theoretically in [37, 60, 61].

It turns out that the results obtained from the evolution of a system in contact with an environment having the same number of degrees of freedom as itself agree with those of a system in contact with an environment with a much larger number of degrees of freedom than itself. After examining the case in which a single harmonic oscillator (the system) interacts with a single harmonic oscillator (the environment), we extend the results obtained to the case where the same system interacts with an environment which is composed of at least two harmonic oscillators. This extension is necessary if we are to study all possible open dynamics of such a system.

Throughout this dissertation, the Markov approximation is employed. This approximation simply assumes that the final state of a system after a stochastic evolution for a short time only depends on its initial state and not on its history or other parameters. Under this approximation, any correlations between the system and its environment can be neglected. This is a very reasonable assumption for large environments. This approximation gives rise to exponential solutions, which are very natural results of decay equations. Going beyond this approximation is not within the scope of our work.

1.1.2 Wave propagation in left-handed materials

Refraction is perhaps one of the most fundamental phenomena of optics and electromagnetic wave propagation. When a beam of light is incident on an interface between two different materials, its path is deflected depending on the ratio of the refractive indices n_1 and n_2 of the two materials. The refractive index of a medium measures how fast it transmits light and how light is bent on entering the material from another medium. The higher the ratio of the indices of refraction of the two media, the slower the propagation and the stronger the deflection. The basis of lenses and imaging lies in the phenomenon of refraction, as any material with an index different than that of its environment will deflect any incoming ray that is not normal to the interface.

In addition to the refractive index, the electric permittivity ϵ and magnetic permeability μ are commonly used material parameters that describe how materials polarize in the presence of electric and magnetic fields. The electric permittivity determines a material's response to an applied electric field, while the magnetic permeability summarizes how the material reacts to an applied magnetic field. These parameters generally depend on frequency, thus leading to the phenomenon of "dispersion". For wave propagation inside materials found in nature, one assumes positive ϵ and μ. The theoretical implications of materials with simultaneously negative ϵ and μ were first proposed in 1968 by the Russian physicist Victor Veselago, and during the last decade, they have been given a great deal of theoretical and experimental attention. Such novel structures have been given the name "left-handed materials", for reasons to be discussed in Chapter 7.

In the second part of this dissertation, we investigate the behavior of a plane electromagnetic wave incident on left-handed materials from vacuum. We obtain the physically important information by explicitly solving Maxwell's equations and by matching the boundary conditions at the interface. Our main focus concerns the implications of allowing for the possibility of the electromagnetic field to have negative energy. It turns out that once negative energy solutions are accepted, the requirement for frequency dispersion for negative refraction to be observed can be relaxed. We also touch upon the role of group velocity in the context of discussing left-handed materials. For reasons to be seen in Chapter 7, we suggest that any discussion involving it should be carefully reconsidered.

1.2 Outline of this dissertation

This dissertation is organized as follows: in Chapter 2, we review the concepts of stochastic processes in both the classical as well as the quantum realm and introduce the quantum operator approach employed in studying the time evolution of a system undergoing a stochastic process. We discuss the importance of open quantum systems and review a special subclass of stochastic processes that have the Markov property. We devote the last section of this chapter to a brief mention of the master equation approach.

In Chapter 3, we introduce the relaxation-generating model on which the results of this dissertation are based. The three main processes comprising this model are discussed in detail and physically realizable systems that could be described by such a model are introduced.

Two examples involving bipartite spin and harmonic oscillator systems are explicitly solved and analyzed in Chapter 4. The composite system under investigation is taken to be an initially uncoupled set of two subsystems: the physical system of interest and the environment with which this system is in contact. Two important time regimes appearing in these examples are examined, and the physical interpretations and consequences of these models are presented and analyzed in detail.

Chapter 5 is a generalization of the results of Chapter 4 to the case where the number of degrees of freedom of the environment is made larger than that of the physical system of interest. This chapter concludes the first part of our dissertation.

In Chapter 6, we make a transition to quantum optics and discuss the quantization of the electromagnetic field in terms of harmonic oscillators by invoking a normal mode expansion.

In Chapter 7, we introduce left-handed materials and investigate the propagation of waves incident on such media from vacuum by solving Maxwell's equations. We discuss the possibility of allowing the electromagnetic field to have a negative energy density, and discuss the implications resulting from such a possibility.

Chapter 8 is a summary of our results and a discussion of possible future directions.

Chapter 2

Stochastic processes and open systems: an overview

There are many situations in physics where the evolution of a set of variables can be calculated with one hundred percent certainty. For example, in Newtonian mechanics, when given the initial conditions, one can in principle write down the equations of motion which relate the change in position and momentum of a particle, at least for finite times. On the other hand, there are also many situations in physics that are based on probabilistic concepts. Take as an example thermodynamics. The theory of thermodynamics relates the average values of physical quantities such as temperature, polarization, number of particles, and so on, to one another. However, it does not say much about the processes that are occurring microscopically and how these processes affect the overall macroscopic picture.

In order to apply probability theory to the real world, we must introduce the concept of a stochastic, or random variable. By definition, stochastic variables are variables whose values are determined by the outcome of an experiment. In a given situation, a stochastic variable may have any one of a number of values. All we can know about this variable is the probability that a particular value of it will be realized in our experiment. Put another way, the values for the dynamical variables are replaced by their probability distributions.

A stochastic, or random process, is the counterpart to a deterministic process. Instead of dealing with only one possible "reality" of how the process might evolve under time (as is the case, for example, for solutions of an ordinary differential equation), in a stochastic or random process there is some indeterminacy in its future evolution described by probability distributions. This means that even if the initial conditions are known, there are many possibilities the process might go to, but some paths are more probable and others less.

In the simplest possible case, a stochastic process amounts to a sequence of random variables known as a time series. An example of such a situation is a Markov chain. This will be discussed in more detail in Section 2.3. Although the random values of a stochastic process at different times may be independent random variables, in most commonly considered situations they exhibit complicated statistical correlations. Familiar examples of processes modeled as stochastic time series include stock market and exchange rate fluctuations, medical data such as a patient's EKG, EEG, blood pressure or temperature, and random movement such as Brownian motion or random walks.

2.1 Stochastic processes in the quantum realm

The examples given above all involve classical stochastic processes. Quantum stochastic processes were introduced and developed by Sudarshan [69].

In quantum mechanics, the state vector $|\psi\rangle$ of a system completely determines the statistical behavior of a measurement. The state vector language has the shortcmoning that it cannot describe mixed systems. Consider, for example, a "mixed quantum system" prepared by statistically combining two different pure states $|\psi_1\rangle$ and $|\psi_2\rangle$, each with probability 1/2. To represent this statistical mixture of pure states, a probability density operator ρ is introduced. The density matrix formalism was developed independently by Landau and Von Neumann in the 1920's [27, 80]. Density matrices not only portray the probabilistic nature of a quantum system, but they also contain all the physically significant information we can possibly obtain about the ensemble in question. The need for a statistical description via density matrices arises when one considers either an ensemble of systems, or one system when its preparation history is uncertain and one does not know with certainty which pure quantum state the system is in.

A general density matrix, expressed in the basis in which it is diagonal, has the form:

$$\rho = \sum_a p_a |\psi_a\rangle\langle\psi_a|, \tag{2.1}$$

where p_a is the probability to be found in the state $|\psi_a\rangle$, and the projectors $|\psi_a\rangle\langle\psi_a|$ form an orthogonal set. The necessary conditions that need to be satisfied for a finite-dimensional density matrix to be able to describe physical quantities are hermiticity, non-negativity, and unit-trace:

$$\begin{aligned} \rho &= \rho^\dagger \\ x_r^* \rho_{rs} x_s &\geq 0 \\ \mathrm{Tr}[\rho] = \sum_a p_a &= 1. \end{aligned}$$

The condition of hermiticity ensures that the eigenvalues of the density matrix are real, non-negativity ensures that these eigenvalues are positive, and unit-trace ensures that they add up to one. These three conditions allow for the interpretation of the diagonal elements of ρ as probability weights.

If the state of the system is *pure*, the sum in Eq. (2.1) has only one term. Then the density matrix $|\psi\rangle\langle\psi|$ is the projection onto the one-dimensional space spanned by $|\psi\rangle$. A pure density matrix has the property $\rho^2 = \rho$. If the density matrix is not pure, we say that it is *mixed.* Then, there are two or more terms in the sum of Eq. (2.1), and $\rho^2 \neq \rho$. In fact, for a mixed density matrix, $\mathrm{Tr}[\rho^2] = \sum_a p_a^2 < \sum_a p_a = 1$. The quantity $\mathrm{Tr}[\rho^2]$ signifies the "purity" of the density matrix.

The expectation value of any observable M acting on a system can be expressed as:

$$\langle M \rangle = \sum_a p_a \langle \psi_a | M | \psi_a \rangle = \mathrm{Tr}[M\rho],$$

so that we can interpret ρ as describing an ensemble of pure quantum states in which the state $|\psi_a\rangle$ occurs with probability p_a.

The evolution of a state $|\psi(t)\rangle$ in quantum mechanics is given by Schrodinger's equation:

$$\hat{H}(t)|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle,$$

where $\hat{H}$ is the Hamiltonian operator and $\hbar$ is the Planck constant. Given the initial state $|\psi(t_0)\rangle$, the time-evolved state $|\psi(t)\rangle$ can be found from:

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

where:

$$\hat{U}(t, t_0) = \mathcal{T}\left\{ e^{-i/\hbar \int_{t_0}^{t} \hat{H}(t')dt'} \right\}$$

is the time evolution operator, $\hat{H}$ is the Hamiltonian of the system, and $\mathcal{T}$ is the time-ordering operator.

Using the Schrodinger equation, we can write the analogous equation of motion for the density operator. This is given by:

$$i\hbar \frac{\partial}{\partial t} \rho(t) = \left[\hat{H}(t), \rho(t) \right], \tag{2.2}$$

which is the differential form of the equation for the evolution of the density operator:

$$\rho(t) = \hat{U}(t, t_0)\rho(t_0)\hat{U}^{\dagger}(t, t_0). \tag{2.3}$$

Equation (2.2) is the Von Neumann equation [80]. It is the analogue of the deterministic evolution from Hamilton's equations of motion. In this dissertation, we study the dynamics of density matrices as stochastic processes.

2.2 Open quantum systems

If our initial state is pure and this state remains pure under time evolution, it means that the evolution is unitary. This is the case of a *closed* system. The evolution of a closed system is governed by Eq. (2.2). For simplicity, we will assume that the Hamiltonian $\hat{H}$ is time-independent, but the present discussion can be extended to the case of time-dependent Hamiltonians without loss of generality. This formalism allows us to write down the time evolution operator that connects the states of our system at two different times, given by Eq. (2.3). We call this the quantum operator approach to studying the dynamics of a system.

Any physical system which is acted on by an external agency and does not react back to it, is characterized by a unitary time evolution. An example of this type is an ensemble of spin particles and associated magnetic moments in the presence of a magnetic field. However, one is often interested in a physical system forming just part of a larger system, or which is in interaction with a larger system. An example of this situation is seen in paramagnetic relaxation, where a system of spins is interacting with a lattice. Further, one may also be interested in just one, or a few, of the many degrees of freedom of a system. For instance, one may wish to only look at the spin state of a particle scattered by a target possessing spin, irrespective of the distribution of the directions. One assumption in approaching the study of a system's evolution is that it is impossible to have knowledge of all the parameters entering the problem. The part which is known is often treated as the system, while the unknown part is treated as the environment.

Open quantum systems are those in which the state does not evolve in isolation, but is influenced instead by the interaction with its environment. This formalism is employed in this dissertation. The usual case for open quantum systems is that even though the details of the system variables are accessible to us, the details of the effect of the environmental variables on this system are inaccessible. The open quantum system is the combination of the system of interest and the environment with which it interacts.

Open systems are not exclusively quantum mechanical. Take as an example a classical swinging pendulum like that found in some mechanical clocks. Such a pendulum can be thought of as a nearly ideal closed system since it interacts only very slightly with the outside world, mainly through friction. However, to describe the full dynamics of the pendulum's motion and to understand why it eventually ceases to swing, one must incorporate into the problem the damping effects of friction and the imperfections in the suspension mechanism. In a similar fashion, no quantum system is ever perfectly isolated from its environment, and thus never perfectly closed.

Open quantum evolution usually deals with mixed states. For this reason, we will represent the quantum states in our discussion using the density matrix formalism, introduced in Section 2.1.

2.3 The Markov approximation

In this section, we describe the subclass of stochastic processes that have the Markov property. Such processes are very important in physics and chemistry. A Markov process is defined as a stochastic process with the property that for any set of n successive times (i.e., $t_1 < t_2 < \cdots < t_n$), one has:

$$P_{1|n-1}(y_n, t_n | y_1, t_1; \cdots ; y_{n-1}, t_{n-1}) = P_{1|1}(y_n, t_n | y_{n-1}, t_{n-1}).$$

That is, the conditional probability density at t_n, given the value y_{n-1} at t_{n-1}, is uniquely determined and is not affected by any knowledge of the values at earlier times. $P_{1|1}$ is the transition probability. A Markov process is fully determined by the two functions $P_1(y_1, t_1)$ and $P_{1|1}(y_2, t_2 | y_1, t_1)$. The whole hierarchy can be reconstructed from them. This makes Markov processes manageable, which is the reason why they are so useful in many applications.

The oldest and best known example of a Markov process in physics is Brownian motion. A heavy particle is immersed in a fluid of light molecules, which collide with it in a random fashion. As a consequence, the velocity of the heavy particle varies by a large number of small, and supposedly uncorrelated jumps. To facilitate the discussion, the motion is treated as if it were one-dimensional. When the velocity of the heavy particle has a certain value v, there will be, on average, more collisions in front that from behind. Hence, the probability for a certain change δv of the particle's velocity in the next time interval δt depends on v, but not on earlier values of the velocity. Thus, the distribution of the velocity of the heavy particle is described by a Markov process.

Radioactive decay is another example in physics that can be described by a Markov process. For example, an atom of carbon-14 may lose an electron and decay to nitrogen-14. This is a Markov process because the probability of decay does not depend on how old the carbon-14 atom is. A newly formed carbon-14 atom has exactly the same probability of decay in the next second as a very old carbon-14 atom.

Markov processes are also very common in chemistry, and specifically chemical reactions. Consider for example the dissociation of a gas of binary molecules in a reaction of the form:

$$AB \to A + B.$$

Every molecule AB has a certain probability per unit time to be broken up by some collision with another molecule. The change in the concentration between two times t and $t + \Delta t$ has a certain probability distribution which depends on the concentration of the molecules at t but not on previous values of the concentration. In this sense, this process is Markovian.

In going from classical to quantum mechanics, the Markov approximation implies that the microscopic processes entering the transition probabilities of the quantum mechanical state of our system do not depend on their past history but only on that at the present time. An implication that follows from this approximation is that the environment as a whole does not change, and neither do the correlations between it and the system of interest.

The Markov approximation will in general lead to irreversibility by effectively preventing the environment from reacting back on the system. If the environment is of such a nature that it is affected by changes in the system and, in addition, if it passes those effects back to the system, then the evolution becomes non-Markovian. In general, the effect of the environment on the system becomes apparent in higher orders of time [83]. Thus, the Markov approximation is reasonable for short time regimes and does not hold for higher orders of time. In addition, a Markov process on a system with n dynamical variables, when reduced to $m < n$ degrees of freedom, can become non-Markovian. For example, if Brownian motion was reduced to the study of the evolution of coordinates only, non-Markovian effects would become apparent. The study of such effects is beyond the scope of this dissertation. The interested reader can find an extensive discussion of non-Markovian processes in [56] and references thereafter. The remainder of this dissertation will deal exclusively with Markov processes.

2.4 A word on the master equation approach

As a final remark, we conclude this chapter with a brief mention to the theory of master equations. The master equation approach describes quantum dynamics in continuous time using differential equations and is an approach used often by physicists. The main objective of master equations is to describe the time evolution of an open system with a differential equation which properly describes non-unitary behavior. The *Kossakowski-Lindblad equation* or master equation in the *Kossakowski-Lindblad form* is the most general type of a Markovian master equation describing non-unitary (dissipative) evolution of the density matrix ρ that is trace preserving and completely positive for any initial condition. The Kossakowski-Lindblad equation reads:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[\hat{H}, \rho] + \sum_j \left[2\hat{L}_j \rho \hat{L}_j^\dagger - \{\hat{L}_j^\dagger \hat{L}_j, \rho\} \right],$$

where $\hat{H}$ is the system Hamiltonian, $\hat{L}_j$ is the Lindblad operator which represents the coupling of the system to its environment, and $\{x, y\} = xy + yx$ denotes an anticommutator.

In deriving a master equation for a process, it is generally assumed that the system and environment begin in a product state. In order to determine $\hat{L}_j$, one usually begins with a system-environment model Hamiltonian and then makes the Markov approximation.

The master equation approach is less general than the quantum operations formalism. Solving a master equation allows one to determine the time dependence of a density matrix, which means that the result can be written as a quantum operation. The reverse process is not always possible. Quantum operations describe only state changes and thus they can be used to also describe non-Markovian effects, in contrast to the master equation approach. Non-Markovian processes can produce

Markovian master equations, but they will only preserve positivity and thus they will not be of the Kossakowski-Lindblad form. For a detailed discussion of Markovian master equations and their limitations, we refer the interested reader to [18, 25, 28, 32]. See also [56, 63].

Chapter 3

A relaxation-generating model

It is customary to divide physics into two branches: macroscopic physics, which is phenomenological in nature, such as non-equilibrium thermodynamics, and microscopic, or atomic physics, in which the basis and explanation of macroscopic physics is examined. Consider, for example, a container filled with a neutral gas. Macroscopic physics would describe the system in terms of a few macrovariables such as pressure, temperature or density. These variables are directly amenable to measurements. Microscopic physics on the other hand would treat the gas as a collection of N interacting molecules. The microscopic dynamics of this gas manifests itself in the fact that these molecules can scatter off each other at a certain rate when kept in a certain temperature and pressure. If we had knowledge of the molecular dynamics, such as for example the two-body scattering cross sections, we could then derive the ideal gas law in a dilute gas with frequent collisions but no correlations between the particles. In the second half of the 19th century, Maxwell and Boltzmann were the first to realize that the laws of macroscopic physics could be derived from the microscopic dynamics of the system, if statistical considerations were invoked.

The above discussion was mainly aimed at systems in equilibrium. However, the role of statistical mechanics is very important for systems away from equilibrium. Let's consider such a system. Suppose that a thermodynamical system has been prepared initially in an equilibrium state characterized by certain well-defined macrovariables such as temperature, pressure, density, etc. Also suppose that at some time $t = 0$, the system is disturbed externally by applying a temperature gradient or any other external field across it. The system will immediately try to respond and adjust to this external stimulus by evolving toward a new macroscopic state that is compatible with this external constraint. The task of deriving the kinetic equations for non-equilibrium statistical mechanics was initiated by Boltzmann with his famous equation [3].

The problem of describing the approach to equilibrium for systems composed of a large number of interacting particles is a very fundamental one, and one that has been studied extensively through the years. Ever since the classic work of Boltzmann, it has been recognized that not only statistical, but also dynamical considerations play a role in the time evolution of these systems.

In this chapter, we give a brief overview of Boltzmann's collision model and introduce a quantum mechanical version of this model. Both these models can be used to provide a mechanism for generating relaxation. The remainder of this dissertation deals exclusively with the latter model.

3.1 Boltzmann's collision model

Boltzmann was interested in the thermodynamics of gases as derived from the Hamiltonian dynamics of the individual atoms comprising those gases. The main question which troubled Boltzmann was related to the irreversibility seen in thermodynamical systems: if Hamiltonian dynamics give rise to reversible processes, how can the irreversibility seen in thermodynamical systems be explained?

Boltzmann considered a dilute gas of neutral molecules interacting with short-range van der Waals forces. Such a system suggests a number of possible simplifications. First and foremost, Boltzmann neglected triple collisions because he assumed that it would be very unlikely that, once two particles are within their short-range sphere of mutual interaction, a third particle would be there as well during the short-time interval of the two-body encounter.

In addition to this, Boltzmann introduced another important assumption which was referred to by Boltzmann as the *Stosszahlansatz*, and is also known as the "molecular chaos assumption". Under this assumption all two-body encounters in the gas are statistically independent. In other words, no particle in the gas carries any information about a previous encounter and its memory about dynamical correlations from previous collisions is wiped out before a new collision starts. Given a situation where the system of interest is in the presence of an environment, the particles comprising the system interact with the particles comprising the environment only for short periods of time such that the environment only affects the system during this short-time interaction. The environment is the set of all other particles except the system of interest. Boltzmann assumed that, after a collision, the state of the environment is the same as its state before a collision.

Another way of looking at the assumptions invoked in Boltzmann's collision model is the following: every time a system particle collides with an environmental particle, some energy is exchanged but energy conservation ensures that the total energy is conserved. Once the interaction is over, the system particle continues its journey (with its new energy) while the environmental particle is discarded (along with its energy). The assumption here is that the probability of the same environmental particle interacting with the system particle again is very low and can be neglected. Once the interaction is over, the system particle continues its journey until it comes across a new environmental particle with which it collides, and the process is repeated. Each time there is a system-environment interaction, energy is exchanged (causing the system's energy to change), and the environmental particle along with its energy is discarded. Successive collisions of this type will eventually cause the system's state to cease to change and the system will reach thermodynamic equilibrium.

This statistical *Stosszahlansatz* introduces a distinction between the event "before a collision" and the event "after a collision" and is the source of irreversibility in the Boltzmann equation.

3.2 The "Interact-Refresh-Repeat" model

In this section, we present the quantum mechanical analogue to the Boltzmann collision model. This model was originally proposed by Rau [54] and it deals with the loss of quantum information to the environment in an irreversible manner, which is the biggest challenge to scalable quantum computation.

Consider a bipartite system ρ^{SE} composed of two initially uncoupled subsystems ρ^S and ρ^E. Let the subsystem described by ρ^S correspond to the "physical system" of interest, and that described by ρ^E correspond to a second subsystem which, in turn, is in contact with a "reservoir", or "thermal bath". This second subsystem can be thought of as the "environment". The composite system described by ρ^{SE} is considered to be a complete system even though ρ^E is kept in an inexhaustible temperature bath.

If an interaction Hamiltonian is applied to this initially uncorrelated composite system for a characteristic time interval τ, the two subsystems will interact and evolve to two new states $\rho^S(\tau)$ and $\rho^E(\tau)$. In the remainder of this dissertation, we will follow a program in which our system is "refreshed" after each characteristic time interval τ, and the same interaction Hamiltonian is repeatedly applied to it until a new steady state is reached.

As discussed in Chapter 2, the time evolution of a closed quantum system

$\rho(t)$ governed by a time-independent Hamiltonian $\hat{H}$ is given by:

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

where $\hat{U}(t, t_0) = e^{-i\hat{H}(t-t_0)/\hbar}$ is the unitary time evolution operator. Quantum correlations are generated when two such systems are forced to interact through some interaction Hamiltonian $\hat{H}_{int}$.

Now let us suppose that we are interested in studying how the physical system of interest described by ρ^S relaxes when in contact with its environment, described by ρ^E. Although the evolution of ρ^{SE} is unitary, the reduced evolution of ρ^S is in general not unitary [69]. Knowing the form of ρ^S at any time t_1 is not sufficient to predict its form at a future time t_2. To extract the reduced evolution of subsystem 1, we need to first calculate the time evolution of ρ^{SE} and then eliminate the effect of the unwanted part by taking the partial trace of the evolved complete system over the environmental degrees of freedom. Namely:

$$\rho^S(t) = \mathrm{Tr}_E[\hat{U}(t)\rho^{SE}(0)\hat{U}^{\dagger}(t)],$$

where $\rho^{SE}(0) = \rho^S(0) \otimes \rho^E(0)$.

Just like in the Boltzmann collision model, emphasis is given to studying how system 1 relaxes when it is in contact with system 2, or how the system of interest relaxes when it is in contact with its environment. The interaction Hamiltonian is applied to the composite system $\rho^{SE}(0)$ for a constant characteristic time interval τ, interrupted, and then reapplied for another time interval τ to the time-evolved state $\rho^{SE}(\tau) = \rho^S(\tau) \otimes \rho^E(\tau)$, where $\rho^S(\tau) = \mathrm{Tr}_E[\hat{U}(\tau)\rho^{SE}(0)\hat{U}^{\dagger}(\tau)]$, and $\rho^E(\tau) = \rho^E(0)$. This very last statement comes about from the fact that system 2 is assumed to be in contact with an inexhaustible temperature bath, or reservoir, so that any change it may undergo during the time interval τ can be neglected.

In summary, at $t > 0$, a general, constant interaction Hamiltonian is applied to the composite system for a characteristic time interval τ, the system is allowed to interact, it is then"refreshed", and the process is repeated.

The "interaction" process is defined as follows: the two quantum systems $\rho^S(0)$ and $\rho^E(0)$ interact with one another through the interaction Hamiltonian $\hat{H}_{int}$ during a time interval $0 < t < \tau$, where τ is fixed. The "refresh" process is the extraction of the reduced time-evolved quantum part $\rho^S(\tau)$ from the complete system $\rho^{SE}(\tau)$ and the resetting of $\rho^E(\tau)$ back to its initial form (which corresponds to discarding the environmental particle after the interaction in the Boltzmann collision model). Finally, the "repeat" process is the application of the same interaction Hamiltonian to the new state $\rho^{SE}(\tau) = \rho^S(\tau) \otimes \rho^E(\tau)$ $\big($with $\rho^E(\tau) = \rho^E(0)\big)$ for another time interval $\tau < t < 2\tau$.

There are several areas in physics where periodic couplings along with the Markov approximation are reasonable. For example, in spintronics, in the case of paramagnetic relaxation, a system of spins interacts with a lattice, and the information is encoded in the spin states of the conduction electrons [50]. In this case, the conduction electron takes the role of system 1, and the atoms in the lattice take the role of system 2, or the environment. As the conduction electron passes through the lattice, it interacts with a lattice atom, and as a consequence, its state is changed. This new state will now interact with another atom in the lattice, identical to the first one.

The following assumptions are made in the formulation of generating relaxation as described in the "interact-refresh-repeat" model: first, it is assumed that there is statistical independence between the two density matrices of subsystems 1 and 2 at $t = 0$, or in other words, the density matrix of the composite system can be factorized into density matrices of the component subsystems at $t = 0$, i.e., $\rho^{SE}(0) = \rho^S(0) \otimes \rho^E(0)$. Second, the relaxation time of the system of interest, subsystem 1, is much larger than the characteristic interval τ. In other words, the system is reset before the time interval specified by the inverse of the interaction energy. Third, time averages are never taken, but after every characteristic time interval τ, partial trace with respect to the environment is performed. Finally, system 2 is assumed to be in an inexhaustible temperature bath so that any change in it during the interaction process is negligible.

At each time interval τ, the system goes back to its original state at $t = 0$, while system 1, the system of interest, changes its state. The mechanism of refreshing introduced in this model annuls the correlation between the two systems 1 and 2 at every characteristic time interval τ and replaces the time-evolved state of subsystem 2 with an identical copy of its original state. The "refresh" procedure is a very important ingredient in our model and we dedicate the last section of this chapter entirely to understanding the implications associated with it.

Our relaxation-generating model is described in more detail below:

$$\begin{tikzcd}
\rho^{SE}(0) & = \arrow[d, "\hat{U}(\tau)"] & \rho^{S}(0) \otimes \rho^{E}(0) \\
\rho^{SE}(\tau) & = \arrow[d, "\hat{U}(\tau)"] & \rho^{S}(\tau) \otimes \rho^{E}(0) \\
 & \cdots \arrow[d, "\hat{U}(\tau)"] & \\
\rho^{SE}(n\tau) & = & \rho^{S}(n\tau) \otimes \rho^{E}(0).
\end{tikzcd}$$

More specifically:

$$\begin{tikzcd}
\rho^{SE}(0) & = \arrow[d, "\hat{U}(\tau)"] & \rho^{S}(0) \otimes \rho^{E}(0) \\
\rho^{SE}(\tau) & = \arrow[d, "\hat{U}(\tau)"] & \mathrm{Tr}_E\Big[\hat{U}(\tau)\rho^{SE}(0)\hat{U}^{\dagger}(\tau)\Big] \otimes \rho^{E}(0) \\
 & \cdots \arrow[d, "\hat{U}(\tau)"] & \\
\rho^{SE}(n\tau) & = & \mathrm{Tr}_E\Big[\hat{U}(\tau)\rho^{SE}[(n-1)\tau]\hat{U}^{\dagger}(\tau)\Big] \otimes \rho^{E}(0),
\end{tikzcd}$$

with the time evolution operator given by:

$$\hat{U}(\tau) = e^{-i\hat{H}\tau/\hbar}.$$

A flow chart of our model is shown in Fig. 3.1. The iteration process described above is carried out until a new steady state is reached. Our aim is to study the long time behavior of this periodically repeated interaction scheme and understand its effect on the reduced quantum subsystem ρ^{S}.

Decoherence processes can be modeled using the above relaxation-generating model by controlling the strength, duration, and number of system-environemnt interactions.

3.3 The mechanism of refreshing

As promised, we now turn to the mechanism of refreshing, or the “refresh” process, which is perhaps the most crucial part of our relaxation-generating model. Implicit in this mechanism is the assumption, invoked by Pauli [46], that the occupation numbers of the composite system, which correspond to the diagonal elements of the composite density matrix, remain good quantum numbers at all times. In other words, it is assumed that, during the course of time, off-diagonal terms become unimportant. Pauli eliminated them by invoking a “random phase approximation” at all times. This approximation is a serious ingredient in the analysis of our problem and it is perhaps worthwhile to analyze its use in more depth.

3.3.1 The random phase approximation

The disappearance of interferences between a system and its environment leads to an irreversible process. Irreversible, or energy-dissipating processes always involve transitions between quantum states. Such processes are described, at the simplest level, by master or rate equations. The Pauli master equation [46], is the most commonly used model of irreversible processes in simple quantum systems. It can be derived from elementary quantum mechanics and by neglecting off-diagonal terms.

Among other (inessential to our discussion) approximations, the derivation of the Pauli master equation suffers from the restriction that one has to discard any built-up of phase relations by invoking a repeated “random phase” approximation at a series of times at microscopically small intervals. This restriction may find its justification in Van Kampen’s analysis of the problem in deriving the master equation from quantum mechanics [74, 75]. Specifically, Van Kampen observed that, by writing a master equation, one intends to get statements on macroscopically observable properties of (statistically) large systems. In trying to derive a master equation from quantum mechanics, we must therefore first construct, following Pauli, a suitable coarse-graining of phase-space in such a way that the quantities of the statistical theory are only those that can be measured macroscopically. Any coarse-graining automatically introduces irreversibility into the picture. Van Kampen's derivation of the master equation highlights quite explicitly the inherent difficulties of non-equilibrium statistical mechanics.

To derive a master equation, we must postulate a number of (justifiable) mathematical assumptions, unfortunately in most cases without being able to give the explicit criteria on the microscopic dynamics of the system for these assumptions to be valid. The general attitude is that because many large systems evolve smoothly on a macroscopic time scale, microscopic details are most likely not important, and must therefore be suppressed. Further, it is assumed that the evolution of the reduced density matrix is a Markov process. This translates to invoking a repeated random phase approximation, i.e. neglecting or suppressing any dynamical build-up of phases as time evolves. For example, in the case of photon scattering, interference terms connecting different positions become unobservable at the macroscopic body itself, though still existing in the whole system. This was first discussed by Von Neumann in his theory of the measurement process [80]. Another possible physical mechanism which may aid in explaining the validity of this approximation is the interaction of the system with its natural environment. It has been shown [26, 87], that the interaction between the system and its environment causes some interference terms to become unobservable. In relation to this, it has also been argued that the environment surrounding a quantum system can, in effect, monitor some of the system's observables and as a result, the eigenstates of those observables continuously decohere and can behave like classical states [88].

3.3.2 How does the random phase approximation relate to the partial trace?

For the purposes of this discussion, let us assume that both the system and environment are each described by a single quantum harmonic oscillator. In short, the operation of taking a partial trace assumes that there are no fixed phase relationships between the two oscillators, while at the same time, the phase relationships between the number states of each individual oscillator are definite. In addition, the partial trace also assumes that knowledge of the occupation numbers of each mode of the second system is absent and so the average of these occupation numbers is taken. In contrast, a full fledged random phase approximation considers *all* phase relationships to be random. The partial trace does not go that far.

To get an idea of what the random phase approximation means, we can take the following constructive approach. Let us assume that the state of the overall system is a product state of two pure states of each of the two harmonic oscillators, such that:

$$|\Psi_{12}\rangle = |\psi_1\rangle \otimes |\psi_2\rangle,$$

with:

$$\begin{aligned} |\psi_1\rangle &= \sum_{n_1} p_{n_1} e^{-i\theta_{n_1}} |n_1\rangle \\ |\psi_2\rangle &= \sum_{n_2} p_{n_2} e^{-i\theta_{n_2}} |n_2\rangle, \end{aligned}$$

where p_{n_1} and p_{n_2} are real numbers. The bipartite density matrix is given by:

$$\rho = |\Psi_{12}\rangle \otimes \langle\Psi_{12}| = \sum_{n_1,n_2,n_1',n_2'} p_{n_1} p_{n_2} p_{n_1'} p_{n_2'} e^{-i[(\theta_{n_1}-\theta_{n_1'})-(\theta_{n_2}-\theta_{n_2'})]} |n_1, n_2\rangle\langle n_1', n_2'|. \tag{3.1}$$

The random phase approximation assumes that the four phases θ_{n_1}, θ_{n_2}, $\theta_{n_1'}$, and $\theta_{n_2'}$ in Eq. (3.1) are completely random and the effective density matrix describing the system ρ_{eff} is obtained by integrating out the four phases from ρ. The integral from 0 to 2π over the four phases will kill all terms in ρ except those in which $n_1 = n_1'$ and $n_2 = n_2'$, so that $\theta_{n_1} - \theta_{n_1'} = \theta_{n_2} - \theta_{n_2'} = 0$. In other words, the random phase approximation kills off all the off-diagonal terms in ρ and makes ρ_{eff} diagonal.

The partial trace does something which is different from what we described above. In the case of the partial trace, the assumption made is that nothing is known about the second system. In other words, it is assumed that θ_{n_2} and $\theta_{n_2'}$ are completely random and integration over them can be performed. This will kill off any terms in ρ for which $n_2 \neq n_2'$. In addition to this, it is assumed that there is no knowledge of the occupation numbers of each mode of the second subsystem and hence averaging over all possible occupation numbers can be performed by summing over n_2.

Another way of looking at the partial trace is the following. Let as define $\theta_{n_1} - \theta_{n_1'} \equiv \Theta_{n_1 n_1'}$ and $\theta_{n_2} - \theta_{n_2'} \equiv \Theta_{n_2 n_2'}$. If we assume that the phase relationship between the two oscillators given by $\Theta_{n_1 n_1'} - \Theta_{n_2 n_2'}$ is unknown, we can average over this unknown relative phase. This is analogous to integrating Eq. (3.1) over either $\Theta_{n_1 n_1'}$ or $\Theta_{n_2 n_2'}$. If we perform the integration over $\Theta_{n_2 n_2'}$, all terms with $n_2 \neq n_2'$ will be removed. Further sum over n_2 justified by the lack of knowledge of the occupation numbers in the second system leads to the operation of partial trace.

Note that the discussion above assumes that the state $|\Psi_{12}\rangle$ is a pure product state. This will not be the case for the systems considered in the remainder of this dissertation. The density matrix $\rho^{SE}(\tau)$ on which the partial trace is performed is neither pure nor a product state. However, a similar analysis can be extended to the case where $|\Psi_{12}\rangle$ is not a product state and the subsystems $|\psi_1\rangle$ and $|\psi_2\rangle$ are not pure. This example was used because of its transparency in understanding the subtle differences between the random phase approximation and the partial trace operation.

To summarize, the random phase approximation is a transformation:

$$\rho \to \sum_{n_1,n_2} |n_1, n_2\rangle\langle n_1, n_2|\rho|n_1, n_2\rangle\langle n_1, n_2|,$$

with $|n_1, n_2\rangle$ being the orthonormal basis of the total free Hamiltonian. This transformation is linear with respect to ρ, and corresponds to vanishing of off-diagonal terms in ρ. The operation of the partial trace is not quite the same as the random phase approximation. Whereas the partial trace assumes that we have no knowledge of the occupation numbers of each mode in the second subsystem and hence we end up averaging over those occupation numbers, the random phase approximation considers *all* phase relationships to be random.

We will be revisiting the issues presented in this last section in Chapter 4 for the specific case of two interacting harmonic oscillators.

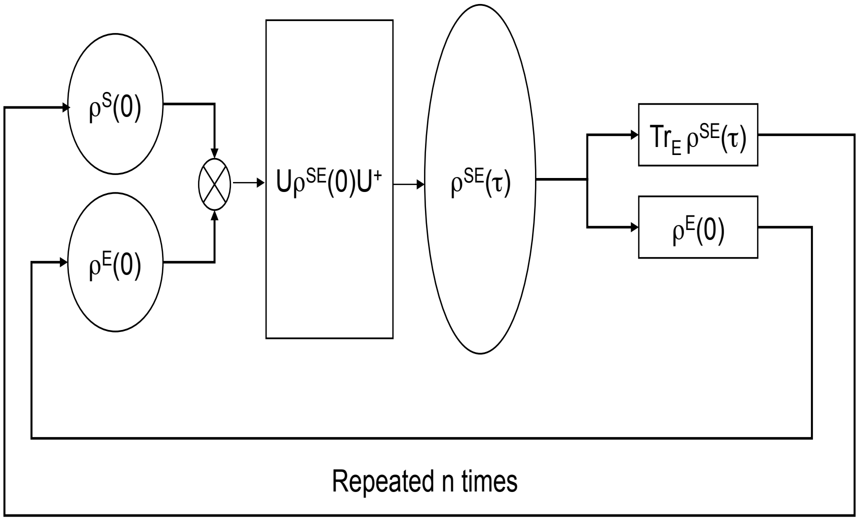

Figure 3.1: Flow Chart describing the first step in the iterative process of "interacting", "refreshing", and "repeating". Two initially uncoupled subsystems are forced to interact through a constant interaction Hamiltonian $\hat{H}_{int}$, the time-evolved composite density matrix is calculated, and the system is "refreshed". Statistical independence is assumed at each characteristic time interval τ. The interaction is again applied to the new uncoupled states of the two subsystems. The process is periodically repeated until a new steady state is reached.

Chapter 4

Dynamics of coupled bipartite systems: some examples

We are now in a position to apply the "interact-refresh-repeat" model to solve some specific examples. We begin with an introduction to the two-state quantum system known as the *qubit* and explicitly solve the open evolution of a bipartite system composed of two such finite-dimensional systems. We continue to extend this calculation to the case involving systems with infinite-dimensional Hilbert spaces, in which case our bipartite system is composed of quantum harmonic oscillators. The physical consequences of the latter case is the main focus of this dissertation.

4.1 An introduction to qubits

The qubit is the basic unit of measurement in quantum information theory. The name "qubit" stands for QUantum BInary digiT. The qubit is analogous to the *bit* (or BInary digiT), which is the basic unit of classical computer information. Irrespective of its physical realization, a bit is always understood to be either a 0 or a 1. Similarly, the two possible computational states of a qubit are the states $|0\rangle$

and $|1\rangle$. The information encoded in a qubit is described by a state vector in a two-level quantum-mechanical system, which is formally equivalent to a two-dimensional Hilbert space.

The qubit has some similarities to the classical bit but is overall very different from it. The main difference is that whereas a bit *must* by either 0 or 1, the qubit can be in state $|0\rangle$, $|1\rangle$, or a linear combination (or superposition) of both:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

where α and β are probability amplitudes and can in general both be complex numbers. α and β are constrained by the equation:

$$|\alpha|^2 + |\beta|^2 = 1, \tag{4.1}$$

where $|\alpha|^2$ is the probability that the qubit is in state $|0\rangle$, and $|\beta|^2$ is the probability that it is in state $|1\rangle$. Geometrically, we can interpret Eq. (4.1) as the condition that the qubit's state be normalized to length 1. Put another way, the state of a qubit is a vector in a two-dimensional complex vector space.

The existence and behavior of qubits has been extensively validated experimentally [39], and there is a plethora of systems found in nature that are physical realizations of these two-level quantum systems. For example, this realization may occur as the two different polarizations of a photon, as the alignment of a nuclear spin in a uniform magnetic field, or as two states ("ground" $|0\rangle$ or "excited" $|1\rangle$) of an electron in the atom model. The electron in the atom model can be moved from the state $|0\rangle$ to the state $|1\rangle$ by shining light on the atom with the appropriate energy and for an appropriate length of time. However, by reducing the time that the light is shone on the atom, the electron can be moved halfway between the states $|0\rangle$ and $|1\rangle$.

4.1.1 Entanglement, or “spooky action at a distance”

An important feature that distinguishes a qubit and a classical bit is that multiple qubits can exhibit *quantum entanglement*. If we had a bipartite system composed of two classical bits, there would be four possible states, 00, 01, 10, and 11. Similarly, a two-qubit system has four computational basis states denoted by $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$. Of-course, a pair of qubits can also exist in a superposition of these four states.

Let’s take as an example two qubits in the state given by:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|00\rangle + |11\rangle\big), \tag{4.2}$$

known as a Bell state. The notation $|ab\rangle$ in Eq. (4.2) translates to the first qubit being in the state $|a\rangle$ and the second qubit being in the state $|b\rangle$. For example, $|00\rangle$ means that both qubits are in the state $|0\rangle$. For the equal superposition state of Eq. (4.2), the probability of measuring $|00\rangle$ or $|11\rangle$ is the same, and equal to $\left|1/\sqrt{2}\right|^2 = 1/2$. This state has the remarkable property that there are no single qubit states $|a\rangle$ and $|b\rangle$ such that $|\psi\rangle = |a\rangle|b\rangle$, or in other words, the state cannot be written as a product of states of its component systems. A state of a composite system that has this property is called an *entangled* state.

Entanglement is specific to the character of quantum systems. It is a nonlocal property that allows a set of qubits to express a higher correlation than is possible in classical systems. This is a real phenomenon which Einstein called “spooky action at a distance”, the mechanism of which cannot, as yet, be explained by any theory; it simply must be taken as given. Quantum entanglement allows qubits that are separated by incredible distances to interact with each other instantaneously, without being limited to the speed of light. Regardless of how great the distance between the correlated particles is, they will remain entangled as long as they are isolated.

If the two entangled qubits of Eq. (4.2) are separated, with one part given to Alice and the other to Bob, and Alice makes a measurement on her qubit obtaining either $|0\rangle$ or $|1\rangle$ with equal probability, Bob must get the exact same measurement as Alice. In other words, if Alice measures a $|0\rangle$, Bob must measure the same, as $|00\rangle$ is the only state where Alice's qubit is a $|0\rangle$.

Many of the successes of quantum computation and communication, such as quantum teleportation and superdense coding, make use of entanglement, suggesting that entanglement is a resource that is unique to quantum computation [39].

Any arbitrary qubit density matrix can be written in the form [39]:

$$\rho = \frac{1}{2}\big(\mathbf{I} + \sum_i a_i\sigma_i\big) = \tfrac{1}{2}\begin{pmatrix} 1+a_3 & a_1 - ia_2 \\ a_1 + ia_2 & 1-a_3 \end{pmatrix}, \tag{4.3}$$

where $\mathbf{I}$ is the 2×2 identity matrix, and the σ_i's are the spin Pauli matrices given by:

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

The a_i's have $i = \{1,2,3\}$, and are real vector components which provide a convenient way of parametrizing single qubit states. The three-dimensional vector $\vec{a}$ is known as the Bloch vector for the state ρ and it satisfies the condition $|\vec{a} \leq 1|$. Its magnitude represents the polarization of the density matrix. The space spanned by Eq. (4.3) can be geometrically interpreted as all the points on or inside the "Bloch sphere", which is the sphere with radius 1 spanned by the a_i's. For example, the case with $|\vec{a} = 1|$ represents a pure state and that with $|\vec{a} = 0|$ represents a fully mixed state. All other cases lie between these two extremums. In calculating the time evolution of a qubit system, we need to calculate the time evolution of its Bloch vector components.

4.2 Dynamics of two coupled spins in the presence of a magnetic field

Our first application of the "interact-refresh-repeat" model of Chapter 3 involves the case of two coupled qubits, mainly because of the calculational simplicity afforded by such systems. For the purposes of the following discussion, we choose to represent a qubit by the two states of a spin-1/2 particle. Without loss of generality, both the system of interest and its environment are represented by a single qubit.

More specifically, our composite system consists of two spin subsystems initially at thermal equilibria at temperatures T_1 and T_2, respectively. Following our model, we assume that spin 2 (the environment) is maintained in an inexhaustible thermal bath at temperature T_2, and that spin 1 is not in contact with any kind of bath. A static external magnetic field H_0 is applied to the system in the z direction. At $t = 0$, the two spin systems are not interacting and the density matrix of the composite system is given by the tensor product of the two subsystems, such that $\rho^{SE}(0) = \rho_1^S(0) \otimes \rho_2^E(0)$. For compactness, we will leave out the superscripts S (for system) and E (for environment), unless the meaning of our discussion is not clear. We are interested in studying the relaxation of the physical system of interest (subsystem 1) when in contact with its environment (subsystem 2), under the successive periodic application of an interaction Hamiltonian.

The free Hamiltonians of this particular system are given by:

$$\begin{aligned} \hat{H}_1 &= \omega_1(\sigma_3 \otimes \mathbf{1}) \\ \hat{H}_2 &= \omega_2(\mathbf{1} \otimes \tau_3), \end{aligned}$$

Here, ω_1 is the precessional frequency of spin 1 in the presence of the magnetic field, and ω_2 is that of system 2. These are determined by the gyromagnetic ratio and the applied external magnetic field. The σ's denote spin Pauli matrices in the Hilbert space of spin system 1, and the τ's denote those matrices in the Hilbert space of spin system 2.

The most general interaction Hamiltonian between the two qubits can be written as:

$$\hat{H}_{int}(t) = \sum_{i,j} \lambda_{ij}(t)(\sigma_i \otimes \tau_j), \tag{4.4}$$

where the subscript indices i, j take values from $\{1, 2, 3\}$, and $\lambda_{ij}(t)$ denotes the strength of coupling between the two spins. By using local unitary transformations [70], Eq. (4.4) can be simplified to:

$$\hat{H}_{int}(t) = \sum_{i} \lambda_i(t)(\sigma_i \otimes \tau_i).$$

For simplicity, we will assume that the coupling parameter $\lambda(t)$ is the same for all three of the possible coupling combinations, i.e., $\lambda_1(t) = \lambda_2(t) = \lambda_3(t)$, and that individual qubits do not evolve freely, such that $\lambda(t) \to \lambda$, and the coupling parameter has no explicit time dependence. With these assumptions, the interaction Hamiltonian (4.4) takes the simplified form:

$$\hat{H}_{int} = \lambda \sum_{i} (\sigma_i \otimes \tau_i). \tag{4.5}$$

From now on, summation over repeated subscript indices will be implied. This choice of the interaction Hamiltonian has no special significance, but it can be shown in [63] that it does not lack any of the important features seen in the evolution of a system under a more general interaction Hamiltonian.

As mentioned above, at $t = 0$, both system and environment are in thermal equilibria at temperatures T_1 and T_2, respectively. This allows for the initial density matrices of the uncoupled systems to be described by Maxwell-Boltzmann statistics, such that:

$$\begin{aligned}\rho^S(0) &= \frac{1}{Z_1}e^{-\hat{H}_1\theta_1} = \frac{1}{Z_1}e^{-\omega_1\theta_1[\sigma_3\otimes\mathbf{1}]}\\ \rho^E(0) &= \frac{1}{Z_2}e^{-\hat{H}_2\theta_2} = \frac{1}{Z_2}e^{-\omega_2\theta_2[\mathbf{1}\otimes\tau_3]}.\end{aligned}$$

The quantity θ is an inverse temperature, defined by $\theta = 1/kT$, where k is the Boltzmann constant. Z is a normalization constant known as the partition function, and it is given by $Z = \sum_n e^{-E_n/(kT)} = \mathrm{Tr}[e^{-\hat{H}/(kT)}]$. In this first illustrative example, we will consider the simplified case where the precessional frequencies of the two spins are the same and equal to that of the interaction Hamiltonian, such that $\omega_1 = \omega_2 = \omega$. This assumption will be relaxed in Section 4.3, but for now, we will employ it in order to simplify the calculation.

The initial density matrix for the composite system is given by:

$$\begin{aligned}\rho^{SE}(0) &= \rho^S(0)\otimes\rho^E(0)\\ &= \frac{1}{Z_1Z_2}e^{-\omega\theta_1[\sigma_3\otimes\mathbf{1}]}e^{-\omega\theta_2[\mathbf{1}\otimes\tau_3]}\\ &= \frac{1}{Z_1Z_2}\Big[(\mathbf{1}\otimes\mathbf{1})\cosh\omega\theta_1 - (\sigma_3\otimes\mathbf{1})\sinh\omega\theta_1\Big]\cdot\\ &\quad\ \big[(\mathbf{1}\otimes\mathbf{1})\cosh\omega\theta_2 - (\mathbf{1}\otimes\tau_3)\sinh\omega\theta_2\big], \qquad (4.6)\end{aligned}$$

where we have used the property $\sigma^2 = \tau^2 = \mathbf{1}$ to arrive at the last expression. Equation (4.6) can be put in the form:

$$\begin{aligned}\rho^{SE}(0) &= \frac{1}{Z_1Z_2}\Big[(\mathbf{1}\otimes\mathbf{1})\cosh\omega\theta_1\cosh\omega\theta_2 - (\mathbf{1}\otimes\tau_3)\cosh\omega\theta_1\sinh\omega\theta_2\\ &- (\sigma_3\otimes\mathbf{1})\sinh\omega\theta_1\cosh\omega\theta_2 + (\sigma_3\otimes\tau_3)\sinh\omega\theta_1\sinh\omega\theta_2\Big]. \qquad (4.7)\end{aligned}$$

The time-evolved density matrix for the composite system after one characteristic interval has passed can be calculated by evaluating the expression:

$$\rho^{SE}(\tau) = \hat{U}(\tau)\rho^{SE}(0)\hat{U}^{\dagger}(\tau),$$

in the interaction picture. Here $\hat{U} = e^{-i\hat{H}_{int}\tau}$. It can be shown in [55] that for the interaction Hamiltonian of Eq. (4.5) we have:

$$\begin{aligned}
\hat{U}(\mathbf{1}\otimes\mathbf{1})\hat{U}^{\dagger} &= \mathbf{1}\otimes\mathbf{1} \\
\hat{U}(\sigma_i\otimes\sigma_i)\hat{U}^{\dagger} &= \sigma_i\otimes\sigma_i \\
\hat{U}(\mathbf{1}\otimes\sigma_i)\hat{U}^{\dagger} &= (\mathbf{1}\otimes\sigma_i)e^{2i\lambda\tau(\sigma_j\otimes\sigma_j+\sigma_k\otimes\sigma_k)} \\
\hat{U}(\sigma_i\otimes\sigma_j)\hat{U}^{\dagger} &= (\sigma_i\otimes\sigma_j)e^{2i\lambda\tau(\sigma_i\otimes\sigma_i+\sigma_j\otimes\sigma_j)},
\end{aligned}$$

with $\{i, j, k\}$ cyclic. Using the above results, the evolution of Eq. (4.7) can be written as:

$$\begin{aligned}
\rho^{SE}(\tau) &= \frac{1}{Z_1Z_2}\Big[(\mathbf{1}\otimes\mathbf{1})\cosh\omega\theta_1\cosh\omega\theta_2 - (\mathbf{1}\otimes\tau_3)\cos^2 2\lambda\tau\cosh\omega\theta_1\sinh\omega\theta_2 \\
&- \frac{1}{2}\sin 4\lambda\tau\cosh\omega\theta_1\sinh\omega\theta_2(\sigma_2\otimes\tau_1 - \sigma_1\otimes\tau_2) \\
&- (\sigma_3\otimes\mathbf{1})\sin^2 2\lambda\tau\cosh\omega\theta_1\sinh\omega\theta_2 - (\sigma_3\otimes\mathbf{1})\cos^2 2\lambda\tau\sinh\omega\theta_1\cosh\omega\theta_2 \\
&- \frac{1}{2}\sin 4\lambda\tau\sinh\omega\theta_1\cosh\omega\theta_2(\sigma_1\otimes\tau_2 - \sigma_2\otimes\tau_1) \\
&- (\mathbf{1}\otimes\tau_3)\sin^2 2\lambda\tau\sinh\omega\theta_1\cosh\omega\theta_2 - (\sigma_3\otimes\tau_3)\sinh\omega\theta_1\sinh\omega\theta_2\Big]. \quad (4.8)
\end{aligned}$$

The reduced density matrix of spin 1 after the first characteristic time interval τ has passed is calculated by taking the partial trace of Eq. (4.8) with respect to the environment:

$$\begin{aligned}\rho^S(\tau) &= \mathrm{Tr}_E\left[\rho^{SE}(\tau)\right] \\ &= \frac{1}{Z_1 Z_2}\left[\frac{1}{2}\mathbf{I}\cosh\omega\theta_1\cosh\omega\theta_2 - \frac{1}{2}\sigma_3\sin^2 2\lambda\tau\cosh\omega\theta_1\sinh\omega\theta_2\right. \\ &- \left.\frac{1}{2}\sigma_3\cos^2 2\lambda\tau\sinh\omega\theta_1\cosh\omega\theta_2\right]. \qquad (4.9)\end{aligned}$$

In obtaining Eq. (4.9), we have used the property:

$$\mathrm{Tr}(\tau_i) = 0.$$

Using the fact that:

$$Z_2 = 2\cosh\omega\theta_2,$$

Eq. (4.9) can be written as:

$$\rho^S(\tau) = \frac{1}{Z_1}\Big[\mathbf{I}\cosh\omega\theta_1 - \sigma_3(\sinh\omega\theta_1\cos^2 2\lambda\tau + \cosh\omega\theta_1\tanh\omega\theta_2\sin^2 2\lambda\tau)\Big]. \quad (4.10)$$

We would like to calculate the state of system 1 after n successive interactions have been applied to our composite system. In other words, we are looking for an expression for $\rho^S(n\tau)$. This can be calculated quite easily for the bipartite system at hand by using the method of iteration.

To calculate the time evolution of our spin system, we need to calculate the time evolution of its Bloch vector components. For this particular example, the Bloch vector components are a measure of the temperature of the system. To begin, we note that $\rho^S(0)$ can be written in the form:

$$\rho^S(0) = \frac{1}{Z_1}\Big[\mathbf{I}\cosh\omega\theta_1 - \sigma_3\sinh\omega\theta_1\Big] = \frac{1}{2}\Big[\mathbf{I} - \sigma_3\tanh\omega\theta_1\Big], \qquad (4.11)$$

where we have used the fact that $Z_1 = 2\cosh\omega\theta_1$. In a similar fashion, $\rho^S(\tau)$ given by Eq. (4.10) can be written as:

$$\rho^S(\tau) = \frac{1}{2}\Big[\mathbf{I} - \sigma_3(\tanh\omega\theta_1\cos^2 2\lambda\tau + \tanh\omega\theta_2\sin^2 2\lambda\tau)\Big]. \tag{4.12}$$

Using Eqs. (4.3), (4.11), and (4.12), we see that:

$$\begin{aligned} a_3(\tau) &= \tanh\omega\theta_1\cos^2 2\lambda\tau + \cosh\omega\theta_1\tanh\omega\theta_2\sin^2 2\lambda\tau \\ &= a_3(0)\cos^2 2\lambda\tau + \cosh\omega\theta_1\tanh\omega\theta_2\sin^2 2\lambda\tau \\ &= a_3(0)A + B, \end{aligned}$$

where:

$$\begin{aligned} a_3(0) &= \tanh\omega\theta_1(0) \\ A &= \cos^2 2\lambda\tau \\ B &= \cosh\omega\theta_1\tanh\omega\theta_2\sin^2 2\lambda\tau. \end{aligned}$$

The next few terms can be calculated by using the same technique:

$$\begin{aligned} a_3(2\tau) &= a_3(\tau)A + B = [a_3(0)A + B]A + B = A^2 a_3(0) + B(A+1) \\ a_3(3\tau) &= a_3(2\tau)A + B = [A^2 a_3(0) + B(A+1)]A + B = A^3 a_3(0) + B(A^2 + A + 1) \\ a_3(4\tau) &= a_3(3\tau)A + B = A^4 a_3(0) + B(A^3 + A^2 + A + 1), \end{aligned}$$

and so on. After n such iterations, the Bloch vector component $a_3(n\tau)$ is found to be:

$$a_3(n\tau) = A^n a_3(0) + \left(\frac{A^n - 1}{A - 1}\right),$$

or:

$$\begin{aligned} a_3(n\tau) &= a_3(0)\cos^{2n}2\lambda\tau + \cosh\omega\theta_1\tanh\omega\theta_2\left(\frac{\cos^{2n}2\lambda\tau - 1}{\cos^2 2\lambda\tau - 1}\right)\sin^2 2\lambda\tau \\ &= a_3(0)\cos^{2n}2\lambda\tau + \cosh\omega\theta_1\tanh\omega\theta_2(1-\cos^{2n}2\lambda\tau). \end{aligned}$$

After a total time $t = n\tau$ has passed, $a_3(n\tau)$ can be written as:

$$\begin{aligned} a_3(t) &= \cos^{2t/\tau}2\lambda\tau[a_3(0) - \cosh\omega\theta_1\tanh\omega\theta_2] + \cosh\omega\theta_1\tanh\omega\theta_2 \\ &= \cos^{2t/\tau}2\lambda\tau[a_3(0)+a_0] - a_0, \end{aligned}$$

or:

$$a_3(t) + a_0 = \cos^{2t/\tau}2\lambda\tau[a_3(0)+a_0], \tag{4.13}$$

with:

$$a_0 = -\cosh\omega\theta_1\tanh\omega\theta_2.$$

At $t = 0$, a_3 is a measure of the temperature of system 1, but for $t > 0$, it becomes a function of both θ_1 and θ_2. It is also interesting to note that $a_3(t)$ depends on two time scales: τ for the short-time regime, and t for the long time-regime. We will be discussing these two different time regimes in more detail in Section 4.3. Equation (4.13) can be written in an exponential form, which is characteristic of a thermodynamic decay:

$$a_3(t) + a_0 = e^{-\gamma t}[a_3(0)+a_0] = e^{-t/T}[a_3(0)+a_0], \tag{4.14}$$

where γ is the decay constant and $T = 1/\gamma$ is the relaxation time of our system.

This relaxation time can be calculated from Eqs. (4.13) and (4.14):

$$\begin{aligned}
\cos^{2t/\tau} 2\lambda\tau &= e^{-t/T} \\
\frac{t}{T} &= \ln(\cos^{-2t/\tau} 2\lambda\tau) \\
T &= \frac{\tau}{\ln(\sec 2\lambda\tau)}. \qquad (4.15)
\end{aligned}$$

Equation (4.15) states that the relaxation time of our two-qubit system is directly proportional to the characteristic time-interval τ. In addition, when the coupling strength λ is zero, $T \rightarrow \infty$ and there is no relaxation. In other words, there is no relaxation unless the subsystems are forced to interact with each other. As the coupling strength increases, so does the rate of relaxation.

The reduced density matrix of spin system 1 is given by:

$$\begin{aligned}
\rho^S(t) &= \frac{1}{Z_1}\Big[\cosh\omega\theta_1 - a_3(t)\sigma_3\Big] \\
&= \frac{1}{Z_1}\Big[\cosh\omega\theta_1 - \sigma_3\Big(e^{-t/T}\big(a_3(0)+a_0\big) - a_0\Big)\Big]. \qquad (4.16)
\end{aligned}$$

Letting $t \rightarrow \infty$ in Eq. (4.16) gives:

$$\begin{aligned}
\rho^S(t) &= \frac{1}{Z_1}\Big[\cosh\omega\theta_1 + \sigma_3 a_0\Big] \\
&= \frac{1}{Z_1}\Big[\cosh\omega\theta_1 - \sigma_3\cosh\omega\theta_1\tanh\omega\theta_2\Big] \\
&= \frac{1}{2\cosh\omega\theta_1}\Big[\cosh\omega\theta_1 - \sigma_3\cosh\omega\theta_1\tanh\omega\theta_2\Big] \\
&= \frac{1}{2}\Big[\mathbf{I} - \sigma_3\tanh\omega\theta_2\Big] \\
&= \frac{1}{2\cosh\omega\theta_2}\Big[\cosh\omega\theta_2 - \sigma_3\sinh\omega\theta_2\Big] \\
&= \frac{1}{Z_2}e^{-\hat{H}_1\theta_2}. \qquad (4.17)
\end{aligned}$$

Equation (4.17) states that after a long enough time and after sufficient refreshing intervals, subsystem 1 attains the temperature of the thermal bath that it is in contact with. This result is nothing but a statement of the zeroth law of thermodynamics, and was first noted by Rau [54].

Notice that Eq. (4.12) is characterized by an oscillatory behavior. The interaction Hamiltonian exchanges the system with the environment at periodic intervals without any loss of information or dissipation. However, a system interacts with its environment in an irreversible manner. So how can this irreversibility be understood? The answer to this question can be found in the assumptions put forth in employing the "interact-refresh-repeat" model along with the Markov approximation. The environment is modeled as a stream of identical thermal spins, each interacting independently with the system for a short average time. Decoherence and irreversibility are introduced by the assumption that this interaction is interrupted before there is time for the system to return the exchanged information to the environment. This is in accordance with the Boltzmann collision model.

4.3 Dynamics of two coupled harmonic oscillators

In Section 4.2, we examined the case of a finite-dimensional quantum mechanical system coupled to a finite-dimensional environment through a general interaction Hamiltonian. In this section, we investigate the case of quantum mechanical systems with infinite-dimensional Hilbert spaces coupled together through a general interaction Hamiltonian. More specifically, our composite system is described by two coupled harmonic oscillators.

Following the discussion presented in Section 4.2, we begin our discussion by considering a set of two initially uncoupled harmonic oscillators 1 and 2, described by density matrices $\rho^S(0)$ and $\rho^E(0)$, respectively. Harmonic oscillator 2 acts as the environment, and it is kept at an inexhaustible temperature bath at temperature T_2 at all times, while harmonic oscillator 1 is not in contact with any bath. At $t = 0$, the two oscillators are put in contact, and oscillator 1 relaxes away from its initial equilibrium state. The free and interaction Hamiltonians of our system are given by[1]:

$$\begin{aligned}
\hat{H}_1 &= \hbar\omega_1 \hat{a}_1^\dagger \hat{a}_1 \\
\hat{H}_2 &= \hbar\omega_2 \hat{a}_2^\dagger \hat{a}_2 \\
\hat{H}_{int} &= \hbar\omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1),
\end{aligned}$$

where $\omega_{\{1,2\}}$ is the oscillation frequency of oscillator $\{1,2\}$, and ω is the frequency of the applied interaction Hamiltonian. λ is the constant strength of coupling between the two oscillators. Here, $\hat{a}_1^\dagger$ and $\hat{a}_1$ are the raising and lowering operators for oscillator 1, and similarly, $\hat{a}_2^\dagger$ and $\hat{a}_2$ are the raising and lowering operators for oscillator 2. For simplicity, we set $\hbar = 1$ for the remainder of this thesis.

The interaction Hamiltonian introduces a coupling between the two oscillators through the coupling parameter λ. At the same time, when one quantum is created in one of the oscillators, one quantum is destroyed in the other. This conserves the total number of particles in the two oscillators.

Note that in the coupled spin system example, we limited our attention to the special case where the precessional frequencies of the two subsystems were equal. As promised, we now relax this limiting simplification and explore the case where each oscillator is characterized by its own frequency. We will see that relaxing the equal frequency assumption gives rise to some very interesting physical phenomena.

Just like in the coupled spins case, the initial uncoupled and combined density matrices of the system under consideration are characterized by the Maxwell-

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[1] For a more detailed discussion on the quantum harmonic oscillator, see Chapter 6

Boltzmann distribution and are given by:

$$\begin{aligned}
\rho^S(0) &= \frac{1}{Z_1[\theta_1(0)]} e^{-\omega_1 \hat{a}_1^\dagger \hat{a}_1 \theta_1(0)} && (4.18)\\
\rho^E(0) &= \frac{1}{Z_2[\theta_2(0)]} e^{-\omega_2 \hat{a}_2^\dagger \hat{a}_2 \theta_2(0)} && (4.19)\\
\rho^{SE}(0) &= \rho^S(0) \otimes \rho^E(0)\\
&= \frac{1}{Z_1[\theta_1(0)] Z_2[\theta_2(0)]} e^{-\omega_1 \hat{a}_1^\dagger \hat{a}_1 \theta_1(0)} e^{-\omega_2 \hat{a}_2^\dagger \hat{a}_2 \theta_2(0)}\\
&= \frac{1}{Z_1[\theta_1(0)] Z_2[\theta_2(0)]} e^{-[\omega_1 \hat{a}_1^\dagger \hat{a}_1 \theta_1(0) + \omega_2 \hat{a}_2^\dagger \hat{a}_2 \theta_2(0)]}, && (4.20)
\end{aligned}$$

where we have used the property $[\hat{a}_1^\dagger \hat{a}_1, \hat{a}_2^\dagger \hat{a}_2] = 0$ to obtain the last equation. As before, $\theta_{\{1,2\}} = 1/(kT_{\{1,2\}})$, k is the Boltzmann constant and $T_{\{1,2\}}$ is the initial equilibrium temperature of oscillator $\{1,2\}$. The partition function is given by $Z_i = \sum e^{-E_n/(kT)} = \mathrm{Tr}(e^{-\hat{H}_i/(kT)}) = \mathrm{Tr}(e^{-\omega_i \hat{a}_i^\dagger \hat{a}_i \theta_i})$. We calculate the time evolution of the composite system as before:

$$\begin{aligned}
\rho^{SE}(\tau) &= e^{-i\hat{H}_{total}\tau} \rho^{SE}(0) e^{+i\hat{H}_{total}\tau}\\
&= e^{-i(\hat{H}_1+\hat{H}_2+\hat{H}_{int})\tau} \rho^{SE}(0) e^{+i(\hat{H}_1+\hat{H}_2+\hat{H}_{int})\tau}\\
&= \frac{1}{Z_1[\theta_1(0)] Z_2[\theta_2(0)]} e^{-i\tau[\omega_1 \hat{a}_1^\dagger \hat{a}_1 + \omega_2 \hat{a}_2^\dagger \hat{a}_2 + \omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)]}\\
&\times\ e^{-[\omega_1 \hat{a}_1^\dagger \hat{a}_1 \theta_1(0) + \omega_2 \hat{a}_2^\dagger \hat{a}_2 \theta_2(0)]}\\
&\times\ e^{+i\tau[\omega_1 \hat{a}_1^\dagger \hat{a}_1 + \omega_2 \hat{a}_2^\dagger \hat{a}_2 + \omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)]}. && (4.21)
\end{aligned}$$

To proceed, we note that there is a very interesting connection between the algebra of angular momentum and the algebra of two uncoupled harmonic oscillators. This connection is given by Schwinger's oscillator model of angular momentum [62]. In this model, the following operators are defined:

$$\begin{aligned}
\hat{J}_+ &= \hat{a}_1^\dagger \hat{a}_2 \\
\hat{J}_- &= \hat{a}_2^\dagger \hat{a}_1 \\
\hat{J}_1 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) \\
\hat{J}_2 &= \frac{1}{2i}(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1) \\
\hat{J}_3 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2) \\
j &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2) = \frac{1}{2}(n_1 + n_2) \\
m &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2) = \frac{1}{2}(n_1 - n_2) = \hat{J}_3.
\end{aligned}$$

It can be shown that the above operators satisfy angular momentum commutation relations. With the above definitions, Eq. (4.21) becomes:

$$\begin{aligned}
\rho^{SE}(\tau) &= \frac{1}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]} e^{-i\tau[j(\omega_1+\omega_2)+\hat{J}_3(\omega_1-\omega_2)+2\omega\lambda\hat{J}_1]} \\
&\times \; e^{-j[\omega_1\theta_1(0)+\omega_2\theta_2(0)]-\hat{J}_3[\omega_1\theta_1(0)-\omega_2\theta_2(0)]} \\
&\times \; e^{+i\tau[j(\omega_1+\omega_2)+\hat{J}_3(\omega_1-\omega_2)+2\omega\lambda\hat{J}_1]}.
\end{aligned}$$

Since j commutes with $\hat{J}_1$ and $\hat{J}_3$, we can pull it through and factor it out, obtaining a simplified expression for $\rho^{SE}(\tau)$:

$$\begin{aligned}
\rho^{SE}(\tau) &= \frac{1}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]} e^{-j[\omega_1\theta_1(0)+\omega_2\theta_2(0)]} \times e^{-i\tau[\hat{J}_3(\omega_1-\omega_2)+2\omega\lambda\hat{J}_1]} \\
&\times \; e^{-\hat{J}_3[\omega_1\theta_1(0)-\omega_2\theta_2(0)]} \times e^{+i\tau[\hat{J}_3(\omega_1-\omega_2)+2\omega\lambda\hat{J}_1]}. \qquad (4.22)
\end{aligned}$$

By introducing the parameters:

$$\begin{aligned} a &= \tau(\omega_1 - \omega_2) \\ b &= 2\omega\lambda\tau \\ c &= i[\omega_2\theta_2(0) - \omega_1\theta_1(0)], \end{aligned} \tag{4.23}$$

Eq. (4.22) can be written as:

$$\rho^{SE}(\tau) = \frac{1}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]} e^{-j[\omega_1\theta_1(0)+\omega_2\theta_2(0)]} e^{-i(a\hat{J}_3+b\hat{J}_1)} e^{-ic\hat{J}_3} e^{+i(a\hat{J}_3+b\hat{J}_1)}. \tag{4.24}$$

The reduced time evolution of oscillator 1 after a time τ has passed is obtained by taking the partial trace of Eq. (4.24) over oscillator 2. The matrix elements of such an expression are given by:

$$\begin{aligned} \langle n_1'|\rho^S(\tau)|n_1\rangle &= \sum_{n_2}\langle n_1', n_2|\rho^{SE}(\tau)|n_1, n_2\rangle = \delta_{n_1',n_1}\sum_{n_2}\langle n_1', n_2|\rho^{SE}(\tau)|n_1, n_2\rangle \\ &= \frac{1}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]}\sum_{n_2}\langle n_1, n_2|e^{-j[\omega_1\theta_1(0)+\omega_2\theta_2(0)]} \\ &\times \; e^{-i(a\hat{J}_3+b\hat{J}_1)} \times e^{-ic\hat{J}_3} \times e^{+i(a\hat{J}_3+b\hat{J}_1)}|n_1, n_2\rangle, \end{aligned} \tag{4.25}$$

The appearance of the delta function δ_{n_1',n_1} in Eq. (4.25) is part of the "refresh" procedure presented in Chapter 3 and its meaning will be discussed in detail in Section 4.3.1.

It remains to figure out the action of the exponential operators in Eq. (4.25) on the two-system state $|n_1, n_2\rangle$. This calculation is greatly simplified if we make a transformation to the Euler-angle form $e^{-i\alpha\hat{J}_3}e^{-i\beta\hat{J}_2}e^{-i\gamma\hat{J}_3}$, since the action of the operators $\hat{J}_3$ and $\hat{J}_2$ on this state is a known result. We would like to find expressions for the coefficients α, β, and γ appearing in the Euler-angle form, in terms of the coefficients a, b, and c given by Eq. (4.23). To do this, we make use of the identity:

$$e^{-i\hat{n}\cdot\vec{\sigma}\frac{\phi}{2}} = I\cos\left(\frac{\phi}{2}\right) - i\hat{n}\cdot\vec{\sigma}\sin\left(\frac{\phi}{2}\right),$$

where, for our case:

$$\vec{\sigma} = \sigma_1\hat{\imath} + \sigma_2\hat{\jmath} + \sigma_3\hat{k} = 2\hat{J},$$

(the $\sigma_{\{1,2,3\}}$ are the Pauli spin matrices) and:

$$\hat{n} = \frac{1}{\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2}\right)^2}}\left(\frac{b}{2}\hat{\imath} + \frac{a}{2}\hat{k}\right),$$

such that:

$$\frac{\phi}{2} = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2}\right)^2}.$$

After some extensive but straightforward algebraic calculations, the results are:

$$\begin{aligned}
\alpha &= \arctan\left(\frac{D}{A}\right) + \arctan\left(-\frac{B}{C}\right) \\
\beta &= 2\arccos\left[\frac{A}{\cos\left(\arctan\frac{D}{A}\right)}\right] \\
\gamma &= \arctan\left(\frac{D}{A}\right) - \arctan\left(-\frac{B}{C}\right),
\end{aligned}$$

with:

$$\begin{aligned}
A &= \cos\left(\frac{c}{2}\right) \\
B &= \frac{ab}{2d^2}\sin^2(d)\sin\left(\frac{c}{2}\right) \\
C &= -\frac{b}{d}\cos(d)\sin(d)\sin\left(\frac{c}{2}\right) \\
D &= \left[\cos^2(d) + \frac{\left(\frac{a}{2}\right)^2 - \left(\frac{b}{2}\right)^2}{d^2}\sin^2(d)\right]\sin\left(\frac{c}{2}\right),
\end{aligned}$$

and:

$$d = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2}\right)^2} = \frac{\phi}{2}.$$

With the above transformations, Eq. (4.25) becomes:

$$\begin{aligned}
\langle n_1'|\rho^S(t)|n_1\rangle &= \frac{\delta_{n_1' n_1}}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]}\sum_{n_2}\langle n_1', n_2|e^{-j[\omega_1\theta_1(0)+\omega_2\theta_2(0)]} \\
&\times \; e^{-i\alpha\hat{J}_3}e^{-i\beta\hat{J}_2}e^{-i\gamma\hat{J}_3}|n_1, n_2\rangle \\
&= \frac{1}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]}\sum_{n_2} e^{-\frac{1}{2}(n_1+n_2)[\omega_1\theta_1(0)+\omega_2\theta_2(0)]} \\
&\times \; e^{-\frac{i}{2}(n_1-n_2)(\alpha+\gamma)}\langle n_1, n_2|e^{-i\beta\hat{J}_2}|n_1, n_2\rangle, \qquad (4.26)
\end{aligned}$$

where the $\hat{J}_2$ matrix element in the last equation is given by Wigner's Formula in the $|j, m\rangle$ basis [59]:

$$\begin{aligned}
\langle j, m'|e^{-i\beta\hat{J}_2}|j, m\rangle &= d^{(j)}_{m',m}(\beta) \\
&= \sum_K (-1)^K \frac{\sqrt{(j+m)!(j-m)!(j+m')!(j-m')!}}{(j-m'-K)!K!(j+m-K)!(K+m'-m)!} \\
&\times \; \left(\cos\frac{\beta}{2}\right)^{j+m+j-m'-2K}\left(\sin\frac{\beta}{2}\right)^{2K+m-m'}. \qquad (4.27)
\end{aligned}$$

Substituting Eq. (4.27) into Eq. (4.26) and summing over n_2 and K, we obtain:

$$\begin{aligned}
\langle n_1'|\rho^S(\tau)|n_1\rangle &= \frac{\delta_{n_1', n_1}}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]} \times \left(\frac{1}{1-\cos\left(\frac{\beta}{2}\right)e^{\frac{i}{2}(\alpha+\gamma)-\Theta}}\right) \\
&\times \; \left[\left(\frac{\cos\left(\frac{\beta}{2}\right)}{e^{\Theta+\frac{i}{2}(\alpha+\gamma)}}\right)\left(\frac{1-\sec\left(\frac{\beta}{2}\right)e^{\frac{i}{2}(\alpha+\gamma)-\Theta}}{1-\cos\left(\frac{\beta}{2}\right)e^{\frac{i}{2}(\alpha+\gamma)-\Theta}}\right)\right]^{n_1}, \qquad (4.28)
\end{aligned}$$

where:

$$\Theta = \frac{1}{2}[\omega_1\theta_1(0) + \omega_2\theta_2(0)].$$

Defining $\alpha = i\zeta$ and $\gamma = i\xi$ in Eq. (4.28) and letting $\delta = \frac{1}{2}(\zeta + \xi)$, we finally get:

$$\begin{aligned}\langle n_1'|\rho^S(\tau)|n_1\rangle &= \frac{\delta_{n_1',n_1}}{Z_1[\theta_1(0)]Z_2[\theta_2(0)]}\left[\frac{\cos\left(\frac{\beta}{2}\right)e^{\delta+\Theta}-1}{e^{\Theta-\delta}\left[e^{\Theta+\delta}-\cos\left(\frac{\beta}{2}\right)\right]}\right]^{n_1} \\ &\times \frac{1}{1-\cos\left(\frac{\beta}{2}\right)e^{-(\Theta+\delta)}}. \end{aligned} \tag{4.29}$$

Equation (4.29) can be written in the form:

$$\langle n_1'|\rho^S(\tau)|n_1\rangle = \delta_{n_1',n_1}\frac{1}{Z[\theta_1(\tau)]}e^{-\omega_1 n_1\theta_1(\tau)}, \tag{4.30}$$

with:

$$e^{-\omega_1\theta_1(\tau)} = \frac{\cos\left(\frac{\beta}{2}\right)e^{\Theta+\delta}-1}{e^{\Theta-\delta}\left[e^{\Theta+\delta}-\cos\left(\frac{\beta}{2}\right)\right]}, \tag{4.31}$$

and:

$$Z[\theta_1(\tau)] = Z_1[\theta_1(0)]Z_2[\theta_2(0)]\left[1-\cos\left(\frac{\beta}{2}\right)e^{-(\Theta+\delta)}\right]. \tag{4.32}$$

Equation (4.30) represents a quasi-stationary, non-equilibrium state. It shows that after the interaction Hamiltonian has been applied for a time interval τ, the original Maxwell-Boltzmann distribution describing oscillator 1 with temperature $T_1(0) = 1/[k\theta_1(0)]$ at $t = 0$, is replaced by another Maxwell-Boltzmann distribution and a different temperature $T_1(\tau) = 1/[k\theta_1(\tau)]$, given by Eqs. (4.31) and (4.32). More specifically, the interaction has forced the oscillator out of its initial thermal equilibrium at temperature $T_1(0)$ and brought it to a new thermal equilibrium at temperature $T_1(\tau)$. Once the system has been "refreshed", the interaction process is repeated. The new state of the physical system of interest, $\rho^S(\tau)$, interacts with an identical copy of the initial state of the environment, $\rho^E(0)$.

In the case of the bipartite spin system of Section 4.2, $\rho^S(n\tau)$ was obtained analytically through an iteration method. Unfortunately, in the case of the two oscillators, there is no such simple analytical technique that can be used to obtain $\rho^S(n\tau)$. Technically, of-course, now that we have an expression for the matrix elements of the reduced time-evolved density matrix of oscillator 1 at time τ, our calculations could be repeated to obtain $\langle n_1'|\rho^S(2\tau)|n_1\rangle$, which will lead to another Maxwell-Boltzmann distribution (and another quasi-stationary, non-equilibrium state), with a different temperature $T_1(2\tau) = 1/[k\theta_1(2\tau)]$. The same process can be repeated further to obtain $\langle n_1'|\rho^S(3\tau)|n_1\rangle$, $\langle n_1'|\rho^S(4\tau)|n_1\rangle$, $\cdots$, $\langle n_1'|\rho^S(n\tau)|n_1\rangle$ with an increasing level of difficulty. We bypass the complexity of the analytical method by carrying out the iteration numerically using Mathematica. The graphs of our results are presented in Section 4.3.2.

4.3.1 The delta-function in the reduced density matrix

As promised, we now turn our discussion to the appearance of the delta function in Eq. (4.25). To begin, we note that the reduced density matrix $\rho^S(\tau)$ is diagonal in the number basis $\{|n_1\rangle\}$ of the first harmonic oscillator. This is due to the fact that $j = \hat{N} = 1/2(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2)$ is a conserved quantity in our model ($[\hat{H}, \hat{N}] = 0$), and also because the initial composite density matrix $\rho^{SE}(0) = \rho^S(0) \otimes \rho^E(0)$ is diagonal in the number basis $\{|n_1, n_2\rangle\}$ of the two harmonic oscillators. The only non-zero matrix elements of the bipartite density matrix $\rho^{SE}(\tau)$ at time τ are:

$$\langle n_1', n_2'|\rho^{SE}(\tau)|n_1'', n_2''\rangle,$$

such that $n_1' + n_2' = n_1'' + n_2''$ ($j = j'$), provided that $\rho^{SE}(0)$ had no non-zero matrix elements with $n_1' + n_2' \neq n_1'' + n_2''$.

The evolution generated by the interaction Hamiltonian cannot change the value of the conserved quantity. To make this statement more transparent, we note that the initial, diagonal density operator can be written as:

$$\rho^{SE}(0) = \sum_{n_1,n_2} p_{n_1 n_2} |n_1, n_2\rangle\langle n_1, n_2|,$$

with $n_1, n_2 = 0, 1, 2, \cdots, \infty$. The unitary operator $\hat{U} = e^{-i\hat{H}\tau}$ transforms each operator in the sum above to:

$$|n_1, n_2\rangle\langle n_1, n_2| \to u_{n_1' n_2' n_1'' n_2''} |n_1', n_2'\rangle\langle n_1'', n_2''| \delta_{n_1'+n_2', n_1+n_2} \delta_{n_1''+n_2'', n_1+n_2}.$$

The two delta functions ensure that $n_1 + n_2$ is a conserved quantity under the evolution generated by $\hat{H}$. In addition, the two delta functions together imply that $n_1' + n_2' = n_1'' + n_2''$ in all the terms appearing in $\rho^{SE}(\tau)$. In other words, if $\rho^{SE}(0)$ had no support on operators of the form $|n_1', n_2'\rangle\langle n_1'', n_2''|$ with $n_1' + n_2' \neq n_1'' + n_2''$ to begin with, then the evolution cannot generate support on such terms. Of-course, if the initial density matrix $\rho^{SE}(0)$ had non-zero matrix elements with $n_1' + n_2' \neq n_1'' + n_2''$, then the above argument would not work. The latter situation is beyond the scope of this dissertation.

The partial trace operation assumes that we consider the relative phase between systems 1 and 2 to be completely randomized and thus we can integrate over it. In addition to this, we assume that we know nothing about the occupation numbers of each mode of the second system and hence we can sum over them when computing the partial density matrix of system 1. This produces a $\rho^S(\tau)$ that is diagonal because in performing the partial trace, we set $n_2' = n_2''$ which means that all the terms in $\rho^{SE}(\tau)$ contributing to the partial trace also have $n_1' = n_1''$, since $n_1' + n_2 = n_1'' + n_2$ which leads to $n_1' = n_1''$. Then indeed:

$$\langle n_1' | \rho^S(\tau) | n_1 \rangle = \sum_{n_2} \langle n_1', n_2 | \rho^{SE}(\tau) | n_1, n_2 \rangle = \delta_{n_1, n_1'} \sum_{n_2} \langle n_1', n_2 | \rho^{SE}(\tau) | n_1, n_2 \rangle.$$

It turns out that, for the specific system considered here, there is no need to invoke the random phase approximation to kill off the off-diagonal elements in $\rho^{SE}(\tau)$. Even without this approximation, the answer is the same. This is due to the extra symmetry of our system. In general, if we had chosen a different system with no extra symmetry like this one, the refresh procedure as defined using the partial trace and the random phase approximation would lead to different partial density matrices. Again, this situation is beyond the scope of this dissertation.

4.3.2 Physical interpretation and consequences

The question we want to answer now is: *When is equilibrium achieved*, or *When does the relaxing system reach a steady state*? To answer this question, let's consider the system composed of some energy state $|n_1\rangle$ in oscillator 1 and some energy state $|n_2\rangle$ in oscillator 2. A steady state will be reached when the net rate of "absorption" equals the net rate of "emission" in and out of this system. "Emission" results from transitions such as $|n_1\rangle \rightarrow |n_1+1\rangle$ or $|n_1\rangle \rightarrow |n_1-1\rangle$ in oscillator 1, and $|n_2\rangle \rightarrow |n_2-1\rangle$ or $|n_2\rangle \rightarrow |n_2+1\rangle$ in oscillator 2. Likewise, "absorption" processes are caused from transitions such as $|n_1-1\rangle \rightarrow |n_1\rangle$ or $|n_1+1\rangle \rightarrow |n_1\rangle$ and $|n_2+1\rangle \rightarrow |n_2\rangle$ or $|n_2-1\rangle \rightarrow |n_2\rangle$.

Recalling that $\hat{H}_{int} = \omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)$, we can calculate the probability amplitudes for "emission" out of this bipartite system:

$$\begin{aligned}\langle n_1+1, n_2-1|\omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)|n_1, n_2\rangle &= \omega\lambda\sqrt{n_2(n_1+1)},\\ \langle n_1-1, n_2+1|\omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)|n_1, n_2\rangle &= \omega\lambda\sqrt{n_1(n_2+1)}.\end{aligned}$$

Similarly, the probability amplitudes for "absorption" are given by:

$$\begin{aligned}\langle n_1, n_2|\omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)|n_1-1, n_2+1\rangle &= \omega\lambda\sqrt{n_1(n_2+1)},\\ \langle n_1, n_2|\omega\lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)|n_1+1, n_2-1\rangle &= \omega\lambda\sqrt{n_2(n_1+1)}.\end{aligned}$$

At equilibrium, we expect that:

$$\begin{aligned} P(n_1, n_2)[n_2(n_1+1)] + P(n_1, n_2)[n_1(n_2+1)] &= P(n_1-1, n_2+1)[n_1(n_2+1)] \\ &+ P(n_1+1, n_2-1)[n_2(n_1+1)], \end{aligned} \tag{4.33}$$

where $P(n_1, n_2)$ is the probability to have a particle in energy level $|n_1\rangle$ in oscillator 1 and energy level $|n_2\rangle$ in oscillator 2, etc. Simplifying Eq. (4.33) gives:

$$\begin{aligned} P(n_1, n_2)[2n_1n_2 + n_1 + n_2] &= P(n_1-1, n_2+1)[n_1(n_2+1)] \\ &+ P(n_1+1, n_2-1)[n_2(n_1+1)]. \end{aligned} \tag{4.34}$$

The consequences of Eq. (4.34) can now be explored. Recall that the interaction Hamiltonian imposes the condition that the sum of the occupation numbers n_1 and n_2 in states $|n_1\rangle$ and $|n_2\rangle$ respectively, is a constant. Let's call this constant N, such that $n_1 + n_2 = N$. The case $N = 0$ is trivial, it represents the vacuum state. For $N = 1$, there are two possible transition states, $|1, 0\rangle$ and $|0, 1\rangle$. Solving Eq. (4.34) for these two different cases leads to the condition $P(1, 0) = P(0, 1)$. This result is not surprising. It simply states that, at equilibrium, the probability of a transition to the state $|1, 0\rangle$ is the same as that to the state $|0, 1\rangle$. Similarly, for $N = 2$, there are three possible transition states: $|0, 2\rangle$, $|1, 1\rangle$, and $|2, 0\rangle$. This time, Eq. (4.34) yields a more interesting result: $P(0, 2) = P(1, 1) = P(2, 0)$. Since the sum of all probabilities must be unity, each of these probabilities must be equal to 1/3. Repeating this procedure for increasing N, we soon recognize that for any N, there are $N + 1$ different possible states, and the probability of transition to any of them is the same for all and equal to $1/(N + 1)$.

Making use of the above result and employing Eqs. (4.18) and (4.30), we conclude that the new density matrix for the composite system will be of the form:

$$\langle n_1, n_2|\rho^{SE}(\infty)|n_1, n_2\rangle = \frac{1}{N+1} e^{-\omega_1 n_1 \theta_1(\infty)} e^{-\omega_2 n_2 \theta_2(0)}. \tag{4.35}$$

If we define $\nu = n_1 - n_2$, we can rewrite Eq. (4.35) as:

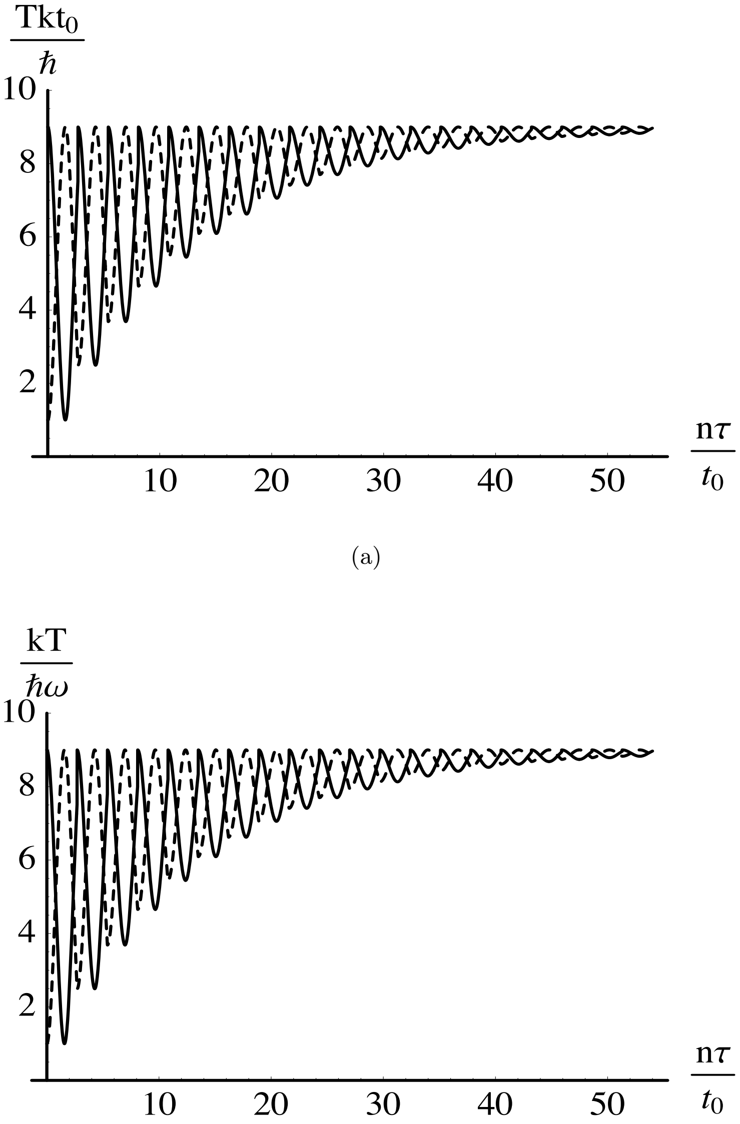
$$\begin{aligned} \langle n_1, n_2|\rho^{SE}(\infty)|n_1, n_2\rangle &= \left\langle \frac{N+\nu}{2}, \frac{N-\nu}{2} \middle| \rho^{SE}(\infty) \middle| \frac{N+\nu}{2}, \frac{N-\nu}{2} \right\rangle \\ &= \frac{1}{N+1} e^{-\omega_1 \left(\frac{N+\nu}{2}\right)\theta_1(\infty)} e^{-\omega_2 \left(\frac{N-\nu}{2}\right)\theta_2(0)} \\ &= \frac{1}{N+1} \left[e^{-\frac{N}{2}\left[\omega_1\theta_1(\infty)+\omega_2\theta_2(0)\right]} e^{-\frac{\nu}{2}\left[\omega_1\theta_1(\infty)-\omega_2\theta_2(0)\right]} \right]. \end{aligned} \tag{4.36}$$

Since, for any N, the probability of transition at equilibrium to any of the $N+1$ possible states is equal to $1/(N+1)$, Eq. (4.36) should be independent of ν. This is true when $e^{-\frac{\nu}{2}[\omega_1\theta_1(\infty)-\omega_2\theta_2(0)]} \to 1$, which leads to the consequence that, at equilibrium, $\omega_1\theta_1(\infty) = \omega_2\theta_2(0)$, or $\omega_1/[kT_1(\infty)] = \omega_2/[kT_2(0)]$.

In the plots below, the "temperature" $(kt_0/\hbar)T$ and the quantity $kT/\hbar\omega$ are plotted as functions of the refreshing time intervals $n\tau/t_0$, for the relaxation of the initial Maxwell-Boltzmann distributions of the two oscillators. Here, we introduce the time constant t_0 for the simplicity of working in a dimensionless system of units. In this system, we set $k = \hbar = t_0 = 1$. The interaction Hamiltonian is applied for a constant time interval τ, interrupted, the system is refreshed, and the procedure is repeated, until oscillator 1 reaches a new steady state. In Figs. 4.1 and 4.2, the frequencies of both harmonic oscillators and that of the interaction Hamiltonian are equal, in Fig. 4.3, the frequencies of the oscillators are equal but that of the interaction Hamiltonian is not, and, finally, in Figs. 4.4 and 4.5, the frequencies of the oscillators and the interaction Hamiltonian are all different. The dashed line represents the evolution of oscillator 1 and the solid one represents the evolution of oscillator 2.

We note some interesting results. The rate with which system 1 reaches a new steady state depends on an interplay between the characteristic time interval τ and the interaction frequency ω. Comparing Figs. 4.1 and 4.2, we observe that, for a constant interaction frequency and a shorter characteristic time interval, harmonic oscillator 1 reaches equilibrium much faster. This can be understood by noting that as τ decreases, the period of the applied interaction Hamiltonian is decreased, and the oscillators do not have as much time to interact before the interaction is interrupted. Decreasing the length of the interaction time prevents the oscillators from returning back the temperature they have exchanged so the equilibrium is achieved faster. In other words, if we let the characteristic time interval τ to be of significant length, the short time behavior tends to dominate. For a longer τ, an overall long time envelope develops. Just like in the example of two interacting spins, this phenomenon begins to suggest exponential decay, a signature of thermodynamic behavior. The same effect is observed when we compare Figs. 4.1 and 4.3: for a constant characteristic time interval and a higher interaction frequency, the oscillators are forced to exchange temperature faster. Again, the equilibrium is attained more quickly.

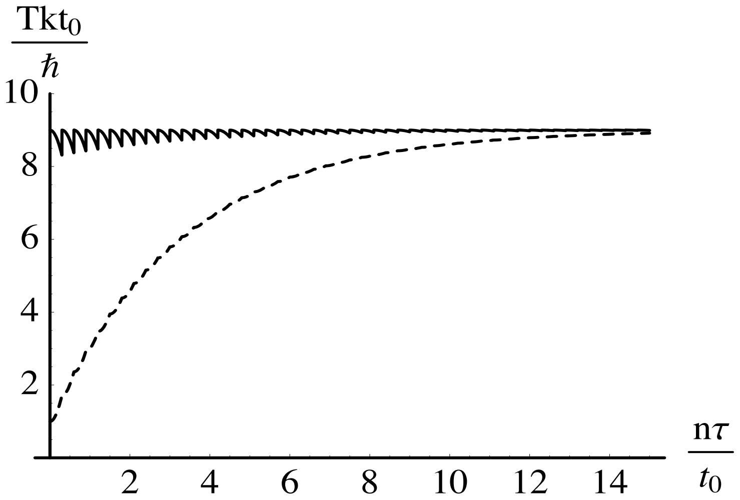
Further, we note that our prediction is verified: $\omega_1\theta_1(\infty) = \omega_2\theta_2(0)$ (or, $\omega_1/[T_1(\infty)] = \omega_2/[T_2(0)]$), at equilibrium. This is shown in subfigures (b) of each figure. In the first three cases, we set $\omega_1 = \omega_2$, and observe that system 1 attains the temperature of its environment as $t \to \infty$. The equilibrium reached is a thermal one, or, in other words, oscillator 1 has reached a steady state where its temperatures has ceased to change, and a single temperature (that of the environment) can be attributed to the composite system. This was in fact noted by several individuals including Montroll and Shuler [35], Mathews, Shapiro, and Falkoff [32], although the problem was solved through a master equation approach and the use of pertur-



(a)

(b)

Figure 4.1: $(kt_0/\hbar)T$ and $kT/\hbar\omega$ as functions of the refreshing time intervals $n\tau/t_0$ for the relaxation of the two initial Maxwell-Boltzmann distributions, with a long characteristic interval τ and equal frequencies. The dashed line represents oscillator 1 and the solid one represents oscillator 2. Here, $k = \hbar = t_0 = 1$, $(kt_0/\hbar)T_1(0) = 1$, $(kt_0/\hbar)T_2(0) = 9$, $\omega_1 t_0 = \omega_2 t_0 = \omega t_0 = 1$, and $\tau/t_0 = 2.7$. The frequencies of the oscillators are the same and system 1 attains a thermal equilibrium with its environment such that $T_1(\infty) = T_2(0)$.



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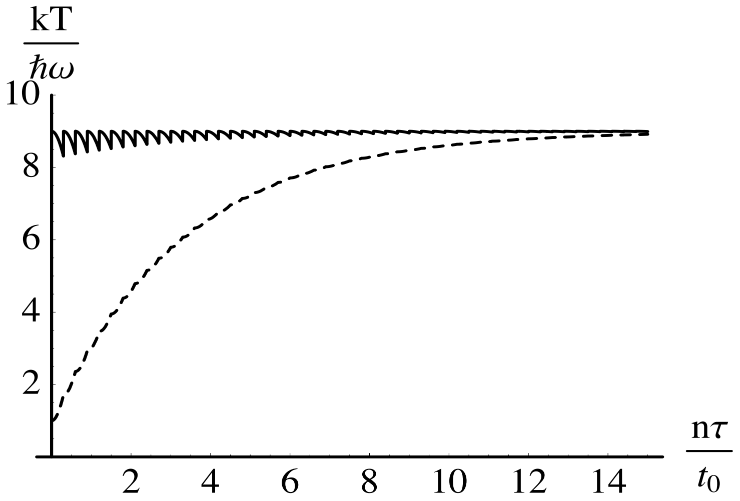
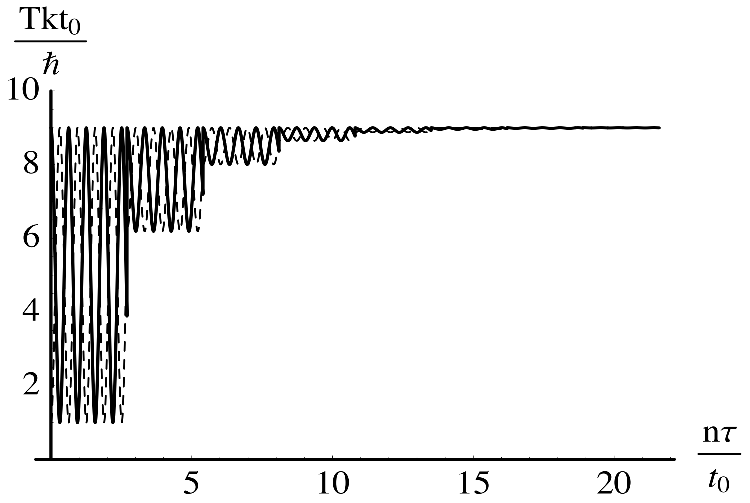


(b)

Figure 4.2: $(kt_0/\hbar)T$ and $kT/\hbar\omega$ as functions of the refreshing time intervals $n\tau/t_0$ for the relaxation of the two initial Maxwell-Boltzmann distributions, with a short characteristic interval τ and equal frequencies. The dashed line represents oscillator 1 and the solid one represents oscillator 2. Here, $k = \hbar = t_0 = 1$, $(kt_0/\hbar)T_1(0) = 1$, $(kt_0/\hbar)T_2(0) = 9$, $\omega_1 t_0 = \omega_2 t_0 = \omega t_0 = 1$, and $\tau/t_0 = 0.3$. Keeping the oscillation frequencies the same as in Fig. 4.1, the characteristic time interval is decreased and thermal equilibrium is reached much faster.



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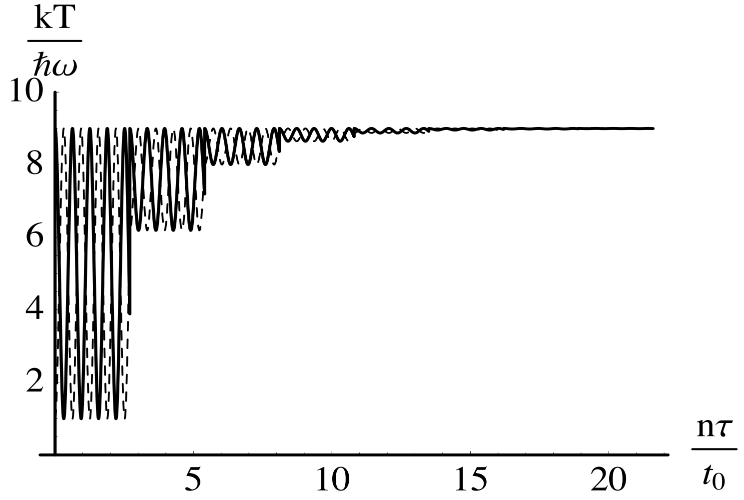
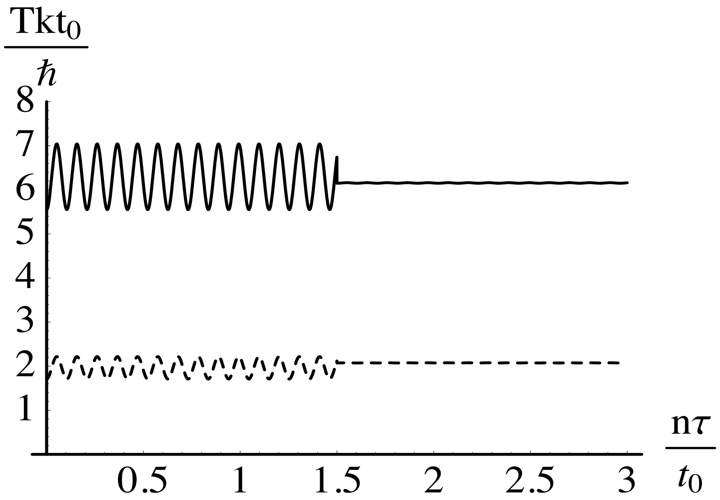
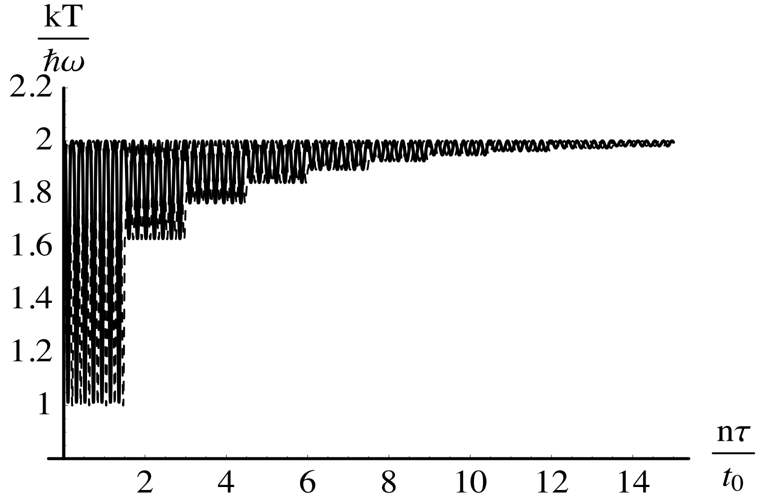


(b)

Figure 4.3: $(kt_0/\hbar)T$ and $kT/\hbar\omega$ as functions of the refreshing time intervals $n\tau/t_0$ for the relaxation of the two initial Maxwell-Boltzmann distributions, with a high interaction frequency ω and equal frequencies. The dashed line represents oscillator 1 and the solid one represents oscillator 2. Here, $k = \hbar = t_0 = 1$, $(kt_0/\hbar)T_1(0) = 1$, $(kt_0/\hbar)T_2(0) = 9$, $\omega_1 t_0 = \omega_2 t_0 = 1$, $\omega t_0 = 5$, and $\tau/t_0 = 2.7$. Keeping the characteristic time interval the same as in Fig. 4.1, the interaction frequency is increased and the equilibrium is reached much faster.

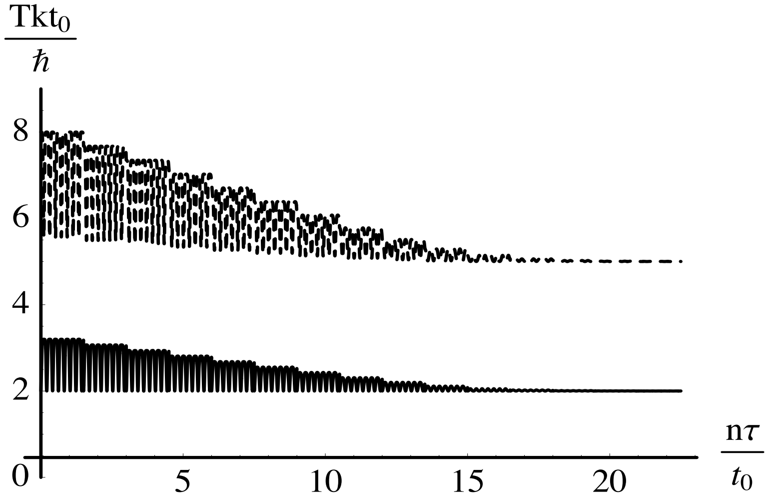


(a)



(b)

Figure 4.4: $(kt_0/\hbar)T$ and $kT/\hbar\omega$ as functions of the refreshing time intervals $n\tau/t_0$ for the relaxation of the two initial Maxwell-Boltzmann distributions with unequal frequencies. The dashed line represents oscillator 1 and the solid one represents oscillator 2. Here, $k = \hbar = t_0 = 1$, $(kt_0/\hbar)T_1(0) = 2$, $(kt_0/\hbar)T_2(0) = 6$, $\omega_1 t_0 = 1$, $\omega_2 t_0 = 3$, $\omega t_0 = 5$, and $\tau/t_0 = 1.5$. Figure (a) shows that oscillator 1 approaches, but does not attain the temperature of its environment, while Fig.(b) demonstrates that the condition $\omega_1/[T_1(\infty)] = \omega_2/[T_2(0)]$ is satisfied.



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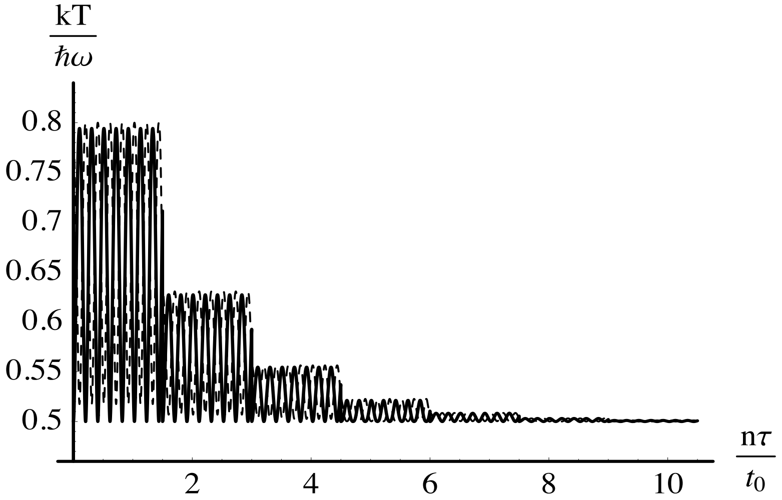

(b)

Figure 4.5: $(kt_0/\hbar)T$ and $kT/\hbar\omega$ as functions of the refreshing time intervals $n\tau/t_0$ for the relaxation of the two initial Maxwell-Boltzmann distributions with unequal frequencies. The dashed line represents oscillator 1 and the solid one represents oscillator 2. Here, $k = \hbar = t_0 = 1$, $(kt_0/\hbar)T_1(0) = 8$, $(kt_0/\hbar)T_2(0) = 2$, $\omega_1 t_0 = 1$, $\omega_2 t_0 = 4$, $\omega t_0 = 5$, and $\tau/t_0 = 1.5$. Again, Fig. (a) shows that oscillator 1 approaches, but does not reach the temperature of its environment, and Fig. (b) shows that the condition $\omega_1/[T_1(\infty)] = \omega_2/[T_2(0)]$ is satisfied.

bation theory. The above result is also in agreement with the results of [54], but the availability of numerical techniques for carrying out the iteration was unavailable at the time. Nonetheless, the predictions made were correct and the results are not surprising. They are simply a consequence of the zeroth law of thermodynamics: when two systems are put in contact with each other, there will be a net exchange of energy between them unless or until they are in thermal equilibrium. This phenomenon has also been studied by Andersen and Shuler for the specific case of the relaxation of a hard-sphere Rayleigh and Lorentz gas [1].

A somewhat more unexpected result (from a thermodynamical point of view), appears in the case where $\omega_1 \neq \omega_2$. The equilibrium reached is not a thermal one and the final composite system no longer satisfies Maxwell-Boltzmann statistics. Oscillator 1 interacts with its environment through the interaction Hamiltonian which takes it out of its initial equilibrium, and eventually reaches a new steady state in which it attains a new equilibrium at a temperature different from that of its environment. While system 1 approaches the temperature of its environment, it never quite reaches it. Its new equilibrium temperature is given by the relation $\omega_1/[T_1(\infty)] = \omega_2/[T_2(0)]$. We note that, besides imposing the condition that the total number of particles is a constant, the interaction Hamiltonian also dictates that the energy of the uncoupled parts of the system (not including the interaction energy) is conserved only when the frequencies of the oscillators are equal:

$$[\hat{H}, \hat{H}_1 + \hat{H}_2] = \omega\lambda(\omega_2 - \omega_1)[\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1],$$

where $\hat{H}_1 + \hat{H}_2$ is the total energy of the uncoupled oscillators without the interaction. The selection rules imposed by the interaction Hamiltonian override the statistical mechanical effects.

The relaxation of our harmonic oscillator system was attained through two equally important parameters: the interaction coupling, introduced through the parameter λ in our interaction Hamiltonian, and a “refresh” procedure, whose mechanism and physical realizations were described in detail in Chapter 3.

Chapter 5

Relaxation through interaction with environments with a larger number of degrees of freedom

In Chapter 4, we studied the approach to equilibrium of a physical subsystem which formed part of a bigger system composed of itself and the environment in which it is in contact with. For what has been presented thus far, the environment has been assumed to be of a size comparable to that of the relaxing physical subsystem. The system composed of a single spin system in Section 4.2 was coupled to an environment composed of only one spin system, and similarly for the harmonic oscillator system of Section 4.3. Realistically, a system will interact with an environment that has a larger number of degrees of freedom than itself.

It turns out that the stochastic evolution of a system in contact with an environment having a larger number of degrees of freedom than itself gives similar results to those of Chapter 4, obtained for the case in which the system is in contact with an environment of similar size. Nonetheless, for the sake of completeness, we would like to generalize the results obtained thus far by examining the case in which the physical system of interest is coupled to a much larger environment. It will be shown that the physical consequences arrived at in Section 4.3 also apply for this more general case.

The physical system of interest will again be modeled by the familiar single harmonic oscillator, but this time, the environment with which it will be in contact with will be a harmonic oscillator chain. As usual, we are interested in how the physical system relaxes when in contact with this environment.

To solve this problem, we will continue to utilize the model presented in Chapter 3. As a reminder of this model's recipe, at $t < 0$ the physical system of interest is uncoupled from the environment, such that the composite system matrix is given by the tensor product of $\rho^S(0)$ and $\rho^E(0)$, where the superscripts S and E denote "system" and "environment", respectively. At $t < 0$, the physical system is at thermal equilibrium at temperature $T_1(0)$, and each degree of the environment described by $\rho_i^E(0)$ is at thermal equilibrium at temperature $T_2(0)$. As per usual, a general interaction Hamiltonian is turned on at $t = 0$, and the physical system couples to its environment.

In what follows, the environment considered is an array of N harmonic oscillators which form a one-dimensional periodic lattice, or a one-dimensional chain. Associated with each harmonic oscillator is a precessional frequency ω_i and a temperature T_2. In all examples to follow, we assume an interaction Hamiltonian that only couples nearest-neighbors. If the physical system of interest is placed at the far left end of the chain and the N^{th} environmental oscillator at the far right and the interaction is turned on, ρ_1^S will couple directly to its nearest neighbor ρ_2^E. Once this happens, both $\rho_1^S(0)$ and $\rho_2^E(0)$ will be taken out of their initial thermal equilibria and this will in turn initiate an interaction between ρ_2^E and ρ_3^E.

The above setup is analogous to the ding-dong model [52] which is a simplified version of the ding-a-ling model [8] in the context of heat conduction. The ding-a-ling model consists of a line of harmonic oscillators with free particles placed between each neighboring harmonic oscillator. In this model, the interaction appears in the form of an elastic collision between the neighboring free particle and the particle of the oscillator. Between collisions, the free particles and the harmonic oscillators move independently. The ding-dong model is the same as the ding-a-ling model but without the free particles. Thus, in this case, the harmonic oscillators can elastically collide with each other.

5.1 Dynamics of a system in contact with an environment composed of two harmonic oscillators: the case of SU(3)

We begin by adding just one additional environmental degree of freedom to the composite system of Section 4.3. More specifically, we consider the case in which the physical system under observation, described as usual by $\rho^S = \rho_1$, is in contact with a bipartite environment $\rho^E = \rho_2 \otimes \rho_3$. The three harmonic oscillators form a chain such that ρ_1 is at the far left end of the chain and ρ_3 is at the far right. All subsystems of this tripartite system are initially uncoupled from one another, such that the initial composite density matrix is given by $\rho^{SE}(0) = \rho^S(0) \otimes \rho^E(0) = \rho_1(0) \otimes [\rho_2(0) \otimes \rho_3(0)]$. As described above, once the interaction is turned on, ρ_1 directly couples to ρ_2. In turn, this interaction initiates a direct coupling between the two environmental oscillators ρ_2 and ρ_3. ρ_1 interacts indirectly with ρ_3 through the direct interaction of ρ_2 with ρ_1 and ρ_3.

The free and interaction Hamiltonians of the composite system are given by:

$$\begin{aligned} \hat{H}_{free} &= \sum_{i=1}^{3} \omega_i \hat{a}_i^\dagger \hat{a}_i & (5.1) \\ \hat{H}_{int}^{SU(3)} &= \omega \sum_{i=1}^{2} g_{i,i+1} \left(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i \right), & (5.2) \end{aligned}$$

where the creation and annihilation operators have their usual meaning. The interaction couplings $g_{i,i+1}$ and the interaction frequency ω are given constants. In the above, we have taken the most general case in which each oscillator is characterized by its own frequency. For simplicity, we restrict our model to the case where $\omega_i = \omega$.

The initial density matrices of the oscillators are characterized by the Maxwell-Boltzmann distribution and are given by:

$$\begin{aligned} \rho^S(0) &= \rho_1(0) \\ &= \frac{1}{Z_1} e^{-\omega \hat{a}_1^\dagger \hat{a}_1 \theta_1} \\ \rho^E(0) &= \rho_2(0) \otimes \rho_3(0) \\ &= \frac{1}{Z_2 Z_3} \sum_{i=2}^{3} e^{-\omega \hat{a}_i^\dagger \hat{a}_i \theta_2} \\ \rho^{SE}(0) &= \rho^S(0) \times \rho^E(0) \\ &= \frac{1}{Z_1 Z_2 Z_3} e^{-\omega \hat{a}_1^\dagger \hat{a}_1 \theta_1} e^{-\omega \theta_2 (\hat{a}_2^\dagger \hat{a}_2 + \hat{a}_3^\dagger \hat{a}_3)} \\ &= \frac{1}{Z_1 Z_2 Z_3} e^{-\omega [\hat{a}_1^\dagger \hat{a}_1 \theta_1 + (\hat{a}_2^\dagger \hat{a}_2 + \hat{a}_3^\dagger \hat{a}_3) \theta_2]}, \end{aligned}$$

where we have used the relation $[\hat{a}_i^\dagger \hat{a}_i, \hat{a}_j^\dagger \hat{a}_j] = 0$ to obtain the last equation.

The density matrix of the composite system after a time interval τ has passed is given by:

$$\rho^{SE}(\tau) = \hat{U}(\tau) \rho^{SE}(0) \hat{U}^\dagger(\tau),$$

where $\hat{U}(\tau) = e^{-i\hat{H}_{total}\tau}$, with $\hat{H}_{total} = \hat{H}_{free} + \hat{H}_{int}$. Following the "interact-refresh-repeat" model of Chapter 3, the effect of the environment will be traced out after each characteristic time interval τ:

$$\rho^S(n\tau) = \mathrm{Tr}_E\Big[\hat{U}(\tau)\rho^{SE}\left[(n-1)\tau\right]\hat{U}^\dagger(\tau)\Big].$$

The time evolution of the composite system is given by:

$$\begin{aligned}
\rho^{SE}(\tau) &= e^{-i\hat{H}_{total}\tau}\rho^{SE}(0)e^{+i\hat{H}_{total}\tau} \\
&= \frac{1}{Z}e^{-i\omega\tau\Big[\sum_{i=1}^{3}\hat{a}_i^\dagger\hat{a}_i + \sum_{i=1}^{2}g_{i,i+1}(\hat{a}_i^\dagger\hat{a}_{i+1}+\hat{a}_{i+1}^\dagger\hat{a}_i)\Big]} \\
&\times\ e^{-\omega\left[\theta_1\hat{a}_1^\dagger\hat{a}_1+\theta_2\sum_{i=2}^{3}\hat{a}_i^\dagger\hat{a}_i\right]} \\
&\times\ e^{+i\omega\tau\Big[\sum_{i=1}^{3}\hat{a}_i^\dagger\hat{a}_i + \sum_{i=1}^{2}g_{i,i+1}(\hat{a}_i^\dagger\hat{a}_{i+1}+\hat{a}_{i+1}^\dagger\hat{a}_i)\Big]},
\end{aligned} \tag{5.3}$$

where the product of the inverse partition functions Z_1, Z_2, and Z_3 has been replaced by $\frac{1}{Z}$.

In the case where the environment was composed of a single harmonic oscillator, we made use of Schwinger's oscillator model in order to connect creation and annihilation operators to the angular momentum algebra. These operators satisfied $SU(2)$ commutation relations. The natural extension of this procedure to the case of a bipartite harmonic oscillator environment is to look for a set of operators satisfying $SU(3)$ commutation relationships.

An $SU(N)$ algebra is generated by N^2-1, linearly independent operators, which satisfy the commutation relationship $[x_i, x_j] = if_{ij}^k x_k$, where the f_{ij}^k are structure constants. An important representation for $N = 3$ involves 3×3 matrices because the group elements act on complex vectors with 3 entries, i.e. on the fundamental representation of the group. A particular choice of this representation is given by the eight Gell-Mann matrices:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

The generators of $SU(3)$ are traceless and Hermitian, and obey the extra relation $\mathrm{Tr}(\lambda_i \lambda_j) = 2\delta_{ij}$. In addition to these matrices, we include the unit matrix which we will call λ_0, for reasons that will become clear later on this chapter:

$$\lambda_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

It is a straight-forward exercise to check that the above $SU(3)$ generators satisfy the required $SU(3)$ commutation relations.

Having obtained the necessary generators, we proceed to constructing the operators of $SU(3)$. Let's call these operators $\hat{K}$'s. Any operator $\hat{K}_i$ can be obtained by calculating the product $\frac{1}{2}\hat{a}^\dagger \lambda_i \hat{a}$, where $\hat{a}^\dagger$ is understood to be a 1×3 row matrix composed of the three raising operators $\hat{a}_1^\dagger, \hat{a}_2^\dagger, \hat{a}_3^\dagger$, and $\hat{a}$ is the corresponding 3×1 column matrix of annihilation operators. In addition to the identity operator, there will be $3^2 - 1$ operators for $SU(3)$. The $\hat{K}$'s are given by:

$$\begin{aligned}
\hat{K}_1 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) \\
\hat{K}_2 &= \frac{1}{2i}(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1) \\
\hat{K}_3 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2) \\
\hat{K}_4 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_3 + \hat{a}_3^\dagger \hat{a}_1) \\
\hat{K}_5 &= \frac{1}{2i}(\hat{a}_1^\dagger \hat{a}_3 - \hat{a}_3^\dagger \hat{a}_1) \\
\hat{K}_6 &= \frac{1}{2}(\hat{a}_2^\dagger \hat{a}_3 + \hat{a}_3^\dagger \hat{a}_2) \\
\hat{K}_7 &= \frac{1}{2i}(\hat{a}_2^\dagger \hat{a}_3 - \hat{a}_3^\dagger \hat{a}_2) \\
\hat{K}_8 &= \frac{1}{2\sqrt{3}}(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 - 2\hat{a}_3^\dagger \hat{a}_3) \\
\hat{K}_0 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 + \hat{a}_3^\dagger \hat{a}_3).
\end{aligned}$$

With these definitions, Eq. (5.3) becomes:

$$\begin{aligned}
\rho^{SE}(\tau) &= \frac{1}{Z} e^{-2i\omega\tau(\hat{K}_0 + g_{12}\hat{K}_1 + g_{23}\hat{K}_6)} \times e^{-\omega\theta_1\left[\frac{1}{3}\left(2\hat{K}_0 + \sqrt{3}\hat{K}_8\right) + \hat{K}_3\right]} \\
&\times \quad e^{-\omega\theta_2\left(\frac{4}{3}\hat{K}_0 - \hat{K}_3 - \frac{1}{\sqrt{3}}\hat{K}_8\right)} \times e^{+2i\omega\tau(\hat{K}_0 + g_{12}\hat{K}_1 + g_{23}\hat{K}_6)},
\end{aligned}$$

where we have used the relations:

$$\begin{aligned}
\hat{a}_1^\dagger \hat{a}_1 &= \frac{2}{3}\hat{K}_0 + \hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 \\
\hat{a}_2^\dagger a_2 &= \frac{2}{3}\hat{K}_0 - \hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 \\
\hat{a}_3^\dagger \hat{a}_3 &= \frac{2}{3}\hat{K}_0 - \frac{2}{\sqrt{3}}\hat{K}_8.
\end{aligned}$$

Since $\hat{K}_0$ commutes with all other operators, we can pull it through and factor it out, obtaining:

$$\begin{aligned}\rho^{SE}(\tau) &= \frac{1}{Z}e^{-\frac{2}{3}\omega\hat{K}_0(\theta_1+2\theta_2)} \times e^{-2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6)} \times e^{-\omega\theta_1\left(\frac{1}{\sqrt{3}}\hat{K}_8+\hat{K}_3\right)} \\ &\times \; e^{+\omega\theta_2\left(\hat{K}_3+\frac{1}{\sqrt{3}}\hat{K}_8\right)} \times e^{+2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6)}.\end{aligned}$$

A final simplification can be made by noting that $\hat{K}_3$ commutes with $\hat{K}_8$:

$$\begin{aligned}\rho^{SE}(\tau) &= \frac{1}{Z}e^{-\frac{2}{3}\omega\hat{K}_0(\theta_1+2\theta_2)} \times e^{-2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6)} \\ &\times \; e^{-\omega(\theta_1-\theta_2)(\hat{K}_3+\frac{1}{\sqrt{3}}\hat{K}_8)}e^{+2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6)}.\end{aligned}$$

The matrix elements of the reduced, time-evolved density matrix are given by:

$$\begin{aligned}\langle n_1'|\rho^S(\tau)|n_1\rangle &= \sum_{n_2,n_3}\langle n_1', n_2, n_3|\rho^{SE}(\tau)|n_1, n_2, n_3\rangle \\ &= \delta_{n_1',n_1}\sum_{n_2,n_3}\langle n_1', n_2, n_3|\rho^{SE}(\tau)|n_1, n_2, n_3\rangle \\ &= \delta_{n_1',n_1}\frac{1}{Z}\sum_{n_2,n_3}\langle n_1', n_2, n_3|e^{-\alpha_{03}\hat{K}_0}e^{-2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6)} \\ &\times \; e^{-\omega(\theta_1-\theta_2)(\hat{K}_3+\frac{1}{\sqrt{3}}\hat{K}_8)}e^{+2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6)}|n_1, n_2, n_3\rangle,\end{aligned}$$

or:

$$\begin{aligned}\langle n_1'|\rho^S(\tau)|n_1\rangle &= \frac{\delta_{n_1',n_1}}{Z}\sum_{n_2,n_3}e^{-\alpha_{03}\frac{N}{2}} \\ &\times \; \langle n_1', n_2, n_3|e^{-2i\omega\tau\hat{H}_{int}^{SU(3)}}e^{-\omega(\theta_1-\theta_2)(\hat{K}_3+\frac{1}{\sqrt{3}}\hat{K}_8)}e^{+2i\omega\tau\hat{H}_{int}^{SU(3)}}|n_1, n_2, n_3\rangle,\end{aligned} \tag{5.4}$$

where:

$$\alpha_{03} = \frac{2}{3}\omega(\theta_1 + 2\theta_2),$$

and the subscript 3 is to remind us that we are in $SU(3)$. The delta function in Eq. (5.4) is introduced for the same reasons as those discussed in Section 4.3.1.

There remains to calculate the action of the interaction Hamiltonian on the state $|n_1, n_2, n_3\rangle$. Let:

$$e^{2i\omega\tau \hat{H}_{int}^{SU(3)}} = e^{2i\omega\tau(g_{12}\hat{K}_1 + g_{23}\hat{K}_6)} = \hat{\Re}^{SU(3)},$$

where the $SU(3)$ superscript is to remind us that we are working in a tripartite composite system. Our task is to calculate $\hat{\Re}^{SU(3)}|n_1, n_2, n_3\rangle$. The state $|n_1, n_2, n_3\rangle$ can be written as:

$$|n_1, n_2, n_3\rangle = \frac{(\hat{a}_1^\dagger)^{n_1}(\hat{a}_2^\dagger)^{n_2}(\hat{a}_3^\dagger)^{n_3}}{\sqrt{n_1!n_2!n_3!}}\Big|0\Big\rangle,$$

and we have:

$$\hat{\Re}^{SU(3)}|n_1, n_2, n_3\rangle = \frac{[\hat{\Re}\hat{a}_1^\dagger\hat{\Re}^{-1}]^{n_1}[\hat{\Re}\hat{a}_2^\dagger\hat{\Re}^{-1}]^{n_2}[\hat{\Re}\hat{a}_3^\dagger\hat{\Re}^{-1}]^{n_3}}{\sqrt{n_1!n_2!n_3!}}\hat{\Re}|0\rangle, \tag{5.5}$$

where we have suppressed the $SU(3)$ superscript on the right hand-side of Eq. (5.5) for compactness. $\hat{\Re}^{SU(3)}$ acting on $|0\rangle$ just reproduces $|0\rangle$, so all we need to do is to calculate the products $\hat{\Re}\hat{a}_1^\dagger\hat{\Re}^{-1}$, $\hat{\Re}\hat{a}_2^\dagger\hat{\Re}^{-1}$, and $\hat{\Re}\hat{a}_3^\dagger\hat{\Re}^{-1}$. At this point, we can use the Baker-Hausdorff lemma:

$$\begin{aligned} e^{i\hat{G}\lambda}\hat{A}e^{-i\hat{G}\lambda} &= \hat{A} + i\lambda[\hat{G},\hat{A}] + \frac{(i\lambda)^2}{2!}\Big[\hat{G},[\hat{G},\hat{A}]\Big] + \\ \cdots &+ \frac{(i\lambda)^n}{n!}\Bigg[\hat{G},\Bigg[\hat{G},\Big[\hat{G},\cdots[\hat{G},\hat{A}]\Big]\Bigg]\cdots\Bigg] + \cdots, \end{aligned}$$

where $\hat{G}$ is a Hermitian operator and λ is a real parameter. Letting $G \rightarrow (g_{12}\hat{K}_1 + g_{23}\hat{K}_6)$, $\lambda \rightarrow 2\omega\tau = a_3$, and $\hat{A} \rightarrow \hat{a}_1^\dagger$, we realize that we must look at various commutators, namely:

$$\begin{aligned}\left[g_{12}\hat{K}_1 + g_{23}\hat{K}_6, a_1^\dagger\right] &= \frac{g_{12}}{2}a_2^\dagger \\ \left[g_{12}\hat{K}_1 + g_{23}\hat{K}_6, \left[g_{12}\hat{K}_1 + g_{23}\hat{K}_6, a_1^\dagger\right]\right] &= \frac{g_{12}}{2}\left[\frac{g_{12}}{2}\hat{a}_1^\dagger + \frac{g_{23}}{2}\hat{a}_3^\dagger\right],\end{aligned}$$

and so forth. Clearly, the commutators will always be proportional to either $a_2^\dagger$ or $\hat{a}_1^\dagger + \hat{a}_3^\dagger$. After quite a bit of algebra, we obtain:

$$\hat{\Re}\hat{a}_1^\dagger\hat{\Re}^{-1} = \hat{a}_1^\dagger\left[1-\frac{g_{12}^2}{2z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right]+i\hat{a}_2^\dagger\left[\frac{g_{12}}{2\sqrt{z}}\sin(a_3\sqrt{z})\right]-\hat{a}_3^\dagger\left[\frac{g_{12}g_{23}}{2z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right], \tag{5.6}$$

where $z = \left(\frac{g_{12}}{2}\right)^2 + \left(\frac{g_{23}}{2}\right)^2$. Following a similar procedure, we get, for the remaining two terms:

$$\begin{aligned}\hat{\Re}\hat{a}_2^\dagger\hat{\Re}^{-1} &= i\hat{a}_1^\dagger\left[\frac{g_{12}}{2\sqrt{z}}\sin(a_3\sqrt{z})\right] + \hat{a}_2^\dagger\left[1 - \frac{a_3^2}{2!}(z-1) - \frac{2}{z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right] \\ &+ i\hat{a}_3^\dagger\left[\frac{g_{23}}{2\sqrt{z}}\sin(a_3\sqrt{z})\right] \qquad (5.7) \\ \hat{\Re}\hat{a}_3^\dagger\hat{\Re}^{-1} &= i\hat{a}_2^\dagger\left[\frac{g_{23}}{2\sqrt{z}}\sin(a_3\sqrt{z})\right] - \hat{a}_1^\dagger\left[\frac{g_{12}g_{23}}{2z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right] \\ &+ \hat{a}_3^\dagger\left[1 - \frac{g_{23}^2}{2z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right]. \qquad (5.8)\end{aligned}$$

Substituting Eqs. (5.6) - (5.8) back into Eq. (5.5) and making use of the Multinomial Theorem:

$$(\hat{a}_1 + \hat{a}_2 + \cdots + \hat{a}_k)^n = \sum_{n_1, n_2, \cdots, n_k \geq 0} \frac{n!}{n_1! n_2! \cdots n_k!}\hat{a}_1^{n_1}\hat{a}_2^{n_2}\cdots\hat{a}_k^{n_k},$$

with $n_1 + n_2 + \cdots + n_k = n$, we obtain:

$$\begin{aligned}
\hat{\Re}^{SU(3)}|n_1, n_2, n_3\rangle &= \sum_{k,l} \Bigg[\frac{n_1! \Big[\hat{a}_1^\dagger \Big[1 - \frac{g_{12}^2}{2z} \sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big) \Big] \Big]^{n_1-k} \Big[i\hat{a}_2^\dagger \Big(\frac{g_{12}}{2\sqrt{z}} \sin(a_3\sqrt{z}) \Big) \Big]^{k-l}}{(n_1-k)!(k-l)!} \\
&\times \frac{\Big[-\hat{a}_3^\dagger \frac{g_{12}g_{23}}{2z} \sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big) \Big]^l}{l!} \Bigg] \\
&\times \sum_{m,\xi} \Bigg[\frac{n_2! \Big[i\hat{a}_1^\dagger \frac{g_{12}}{2\sqrt{z}} \sin(a_3\sqrt{z}) \Big]^{n_2-m} \Big[i\hat{a}_3^\dagger \frac{g_{23}}{2\sqrt{z}} \sin(a_3\sqrt{z}) \Big]^{\xi}}{(n_2-m)!\xi!} \\
&\times \frac{\Big[\hat{a}_2^\dagger \Big[1 - \frac{a_3^2}{2!}(z-1) - \frac{2}{z} \sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big) \Big] \Big]^{m-\xi}}{(m-\xi)!} \Bigg] \\
&\times \sum_{t,p} \Bigg[\frac{n_3! \Big[-\hat{a}_1^\dagger \frac{g_{12}g_{23}}{2z} \sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big) \Big]^{n_3-t} \Big[i\hat{a}_2^\dagger \frac{g_{23}}{2\sqrt{z}} \sin(a_3\sqrt{z}) \Big]^{t-p}}{(n_3-t)!(t-p)!} \\
&\times \frac{\Big[\hat{a}_3^\dagger \Big[1 - \frac{g_{23}^2}{2z} \sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big) \Big] \Big]^{p}}{p!} \Bigg] \Big|0\Big\rangle.
\end{aligned}$$

We would like to compare our expression with:

$$\hat{\Re}^{SU(3)}|n_1, n_2, n_3\rangle = \hat{\Re}^{SU(3)} \Bigg[\frac{(\hat{a}_1^\dagger)^{n_1} (\hat{a}_2^\dagger)^{n_2} (\hat{a}_3^\dagger)^{n_3}}{\sqrt{n_1! n_2! n_3!}} \Big|0\Big\rangle \Bigg]. \tag{5.9}$$

To do this, we factor out the $\hat{a}_1^\dagger$, $\hat{a}_2^\dagger$, and $\hat{a}_3^\dagger$ operators. Our expression becomes:

$$\begin{aligned}
\hat{\mathfrak{R}}^{SU(3)}|n_1, n_2, n_3\rangle &= \sum_{k,l,m,\xi,t,p} \frac{n_1!n_2!n_3!}{(n_1-k)!(n_2-m)!(n_3-t)!} \\
&\times \frac{1}{(k-l)!l!(m-\xi)!\xi!(t-p)!p!} \\
&\times [\hat{a}_1^\dagger]^{n_1-k+n_2-m+n_3-t}[\hat{a}_2^\dagger]^{k-l+m-\xi+t-p}[\hat{a}_3^\dagger]^{l+\xi+p} \\
&\times [-1]^{l+n_3-t}[i]^{k-l+n_2-m+\xi+t-p}\Big[1-\frac{g_{12}^2}{2z}\sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big)\Big]^{n_1-k} \\
&\times \Big[1-\frac{g_{23}^2}{2z}\sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big)\Big]^{p} \\
&\times \Big[\frac{g_{12}g_{23}}{2z}\sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big)\Big]^{l+n_3-t}\Big[\frac{g_{12}}{2\sqrt{z}}\sin(a_3\sqrt{z})\Big]^{k-l+n_2-m} \\
&\times \Big[\frac{g_{23}}{2\sqrt{z}}\sin(a_3\sqrt{z})\Big]^{\xi+t-p}\Big[1-\frac{a_3^2}{2!}(z-1)-\frac{2}{z}\sin^2\Big(\frac{a_3\sqrt{z}}{2}\Big)\Big]^{m-\xi}\Big|0\Big\rangle.
\end{aligned} \tag{5.10}$$

Equating the coefficients of the powers of $\hat{a}_1^\dagger$, $\hat{a}_2^\dagger$, and $\hat{a}_3^\dagger$ in Eqs. (5.9) and (5.10), we identify:

$$\begin{aligned}
n_1-k+n_2-m+n_3-t &= n_1 \\
k-l+m-\xi+t-p &= n_2 \\
l+\xi+p &= n_3,
\end{aligned}$$

from which we obtain the relations:

$$\begin{aligned}
\xi &= n_3-l-p \\
t &= n_2+n_3-k-m.
\end{aligned}$$

The equations above are a statement that the sum over ξ is not independent of the sums over l and p, and similarly, that the sum over t is not independent of the sums over k and m. By taking advantage of these equalities, we can eliminate ξ in favor of

l and p, and t in favor of k and m. After a simple calculation, Eq. (5.10) becomes:

$$\begin{aligned}
\hat{\mathfrak{R}}^{SU(3)}|n_1, n_2, n_3\rangle &= \sum_{k,l,m,p} \frac{n_1! n_2! n_3!}{(n_1-k)!(k-l)!(l)!(n_2-m)!(p)!} \left[\hat{a}_1^\dagger\right]^{n_1} \left[\hat{a}_2^\dagger\right]^{n_2} \left[\hat{a}_3^\dagger\right]^{n_3} \\
&\times \frac{\left[-1\right]^{l-n_2+k+m} \left[i\right]^{2(n_2+n_3-l-p-m)} \left[1-\frac{g_{12}^2}{2z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right]^{n_1-k}}{(m-n_3+l+p)!(n_3-l-p)!(k+m-n_2)!} \\
&\times \frac{\left[1-\frac{g_{23}^2}{2z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right]^{p}}{(n_2+n_3-k-m-p)!} \\
&\times \left[\frac{g_{12}g_{23}}{2z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right]^{l-n_2+k+m} \left[\frac{g_{12}}{2\sqrt{z}}\sin(a_3\sqrt{z})\right]^{k-l+n_2-m} \\
&\times \left[\frac{g_{23}}{2\sqrt{z}}\sin(a_3\sqrt{z})\right]^{2n_3+n_2-2p-l-k-m} \\
&\times \left[1-\frac{a^2}{2!}(z-1)-\frac{2}{z}\sin^2\left(\frac{a_3\sqrt{z}}{2}\right)\right]^{m-n_3+l+p} \Big|0\Big\rangle.
\end{aligned} \tag{5.11}$$

Equation (5.11) can be written in the form:

$$\hat{\mathfrak{R}}^{SU(3)}|n_1, n_2, n_3\rangle = f(n_1, n_2, n_3)|0\rangle,$$

Equation (5.4) then becomes:

$$\langle n_1'|\rho^S(\tau)|n_1\rangle = \frac{\delta_{n_1', n_1}}{Z} \sum_{n_2, n_3} e^{-\alpha_{03}\frac{N}{2}} e^{-\frac{\omega}{3}(\theta_1-\theta_2)(2n_1-n_2-n_3)} |f(n_1, n_2, n_3)|^2, \tag{5.12}$$

with $f(n_1, n_2, n_3)$ given by Eq. (5.11).

In analogy to the single environmental harmonic oscillator case, we expect that the initial Maxwell-Boltzmann distribution of our physical system will be replaced by another Maxwell-Boltzmann distribution at temperature $T_1(\tau)$ after one characteristic interval τ has passed, or in other words, that Eq. (5.12) will be of the form:

$$\langle n_1'|\rho^S(\tau)|n_1\rangle = \frac{\delta_{n_1',n_1}}{Z[\theta_1\tau]}e^{-\omega n_1\theta_1(\tau)}.$$

Theoretically, we should now be able to compute $T_1(2\tau)$, $T_1(3\tau), \cdots, T_1(n\tau)$ by the method of iteration. Unfortunately, there is no simple analytic solution to Eq. (5.11) and thus no simple iterative procedure that will allow us to do so. Nonetheless, we can still get some insight into the conditions which need to be satisfied for ρ^S to reach a new steady state.

Following the discussion of Section 4.3.2, let's consider the energy states $|n_1\rangle$, $|n_2\rangle$, and $|n_3\rangle$, corresponding to oscillators 1, 2, and 3, respectively. At the new equilibrium, the net rate of absorption into this set of states will be equal to the net rate of emission out of it. For the given interaction Hamiltonian of Eq. (5.2), the probabilities of absorption into and emission out of this set of energy states can be calculated. Setting these probabilities equal to each other gives:

$$\begin{aligned} & P(n_1,n_2,n_3)\left[g_{12}^2(2n_1n_2+n_1+n_2)+g_{23}^2(2n_2n_3+n_2+n_3)\right] \\ = \quad & P(n_1+1,n_2-1,n_3)g_{12}^2[n_2(n_1+1)]+P(n_1-1,n_2+1,n_3)g_{12}^2[n_1(n_2+1)] \\ + \quad & P(n_1,n_2+1,n_3-1)g_{23}^2[n_3(n_2+1)]+P(n_1,n_2-1,n_3+1)g_{23}^2[n_2(n_3+1)]. \end{aligned} \tag{5.13}$$

Once again, the interaction Hamiltonian imposes the condition that:

$$n_1+n_2+n_3=N$$

is a constant. In addition, it can be shown from Eq. (5.13) that for any N, there are $(N+2)!/(2!N!)$ possible transition states and that the probability of transition to any one of these states is the same and equal to $(2!N!)/(N+2)!$. Therefore, we can expect that at equilibrium, our composite system will be of the form:

$$\langle n_1, n_2, n_3|\rho^{SE}(\infty)|n_1, n_2, n_3\rangle = \frac{2!N!}{(N+2)!}e^{-\omega n_1\theta_1(\infty)}e^{-\omega(n_2+n_3)\theta_2(0)}. \tag{5.14}$$

If we define $\nu = n_1 - n_2 - n_3$, we can write Eq. (5.14) as:

$$\begin{aligned}\langle n_1, n_2, n_3|\rho^{SE}(\infty)|n_1, n_2, n_3\rangle &= \frac{2!N!}{(N+2)!}e^{-\frac{\omega}{2}(N+\nu)\theta_1(\infty)}e^{-\frac{\omega}{2}(N-\nu)\theta_2(0)} \\ &= \frac{2!N!}{(N+2)!}e^{-\frac{\omega}{2}N\left[\theta_1(\infty)+\theta_2(0)\right]}e^{-\frac{\omega}{2}\nu\left[\theta_1(\infty)-\theta_2(0)\right]}.\end{aligned}$$

The probability of transition to any of the possible states should be independent of ν, and this requires that $e^{-\frac{\omega}{2}\nu\left[\theta_1(\infty)-\theta_2(0)\right]} \to 1$, or that $\theta_1(\infty) = \theta_2(0)$. It can also be shown that if we had allowed for the case $\omega_i \neq \omega$ such that the frequency of ρ^S was ω_1 and that of ρ^E was ω_2, the condition for the new steady state would be $\omega_1\theta_1(\infty) = \omega_2\theta_2(0)$, in agreement to the results of Chapter 4.

5.2 Dynamics of a system in contact with an environment composed of three and four harmonic oscillators

In the previous section, we saw that the addition of even a single environmental degree of freedom makes the solution to our problem significantly more challenging. Before generalizing our results to the case of N environmental harmonic oscillators, it is perhaps insightful to examine the $SU(4)$ and $SU(5)$ cases. As per usual, we will assume the same system-environment model, only each time, an extra environmental degree of freedom will be added. Once again, only nearest-neighbor interactions will be assumed.

5.2.1 The case of $SU(4)$

The free and interaction Hamiltonians for the case where the environment is composed of three harmonic oscillators are given by:

$$\begin{aligned}\hat{H}_{free} &= \omega\sum_{i=1}^{4}\hat{a}_i^{\dagger}\hat{a}_i \\ \hat{H}_{int}^{SU(4)} &= \omega\sum_{i=1}^{3}g_{i,i+1}(\hat{a}_i^{\dagger}\hat{a}_{i+1}+\hat{a}_{i+1}^{\dagger}\hat{a}_i).\end{aligned}$$

The initial density matrices for the system and environment are given by:

$$\begin{aligned}\rho^S(0) &= \frac{1}{Z_1}e^{-\omega\hat{a}_1^{\dagger}\hat{a}_1\theta_1} \\ \rho^E(0) &= \frac{1}{Z_2Z_3Z_4}\sum_{i=2}^{4}e^{-\omega\hat{a}_i^{\dagger}\hat{a}_i\theta_2},\end{aligned}$$

while $\rho^{SE}(\tau)$ is given by:

$$\begin{aligned}\rho^{SE}(\tau) &= \frac{1}{Z}e^{-i\omega\tau\Big[\sum_{i=1}^{4}\hat{a}_i^{\dagger}\hat{a}_i+\sum_{i=1}^{3}g_{i,i+1}(\hat{a}_i^{\dagger}\hat{a}_{i+1}+\hat{a}_{i+1}^{\dagger}\hat{a}_i)\Big]} \\ &\times\ e^{-\omega\Big[\theta_1\hat{a}_1^{\dagger}\hat{a}_1+\theta_2\sum_{i=2}^{4}\hat{a}_i^{\dagger}\hat{a}_i\Big]} \\ &\times\ e^{+i\omega\tau\Big[\sum_{i=1}^{4}\hat{a}_i^{\dagger}\hat{a}_i+\sum_{i=1}^{3}g_{i,i+1}(\hat{a}_i^{\dagger}\hat{a}_{i+1}+\hat{a}_{i+1}^{\dagger}\hat{a}_i)\Big]},\end{aligned}\tag{5.15}$$

with $Z = Z_1Z_2Z_3Z_4$. Following the method used to solve the $SU(2)$ and $SU(3)$ cases, we can utilize the Gell-Mann type basis for the Lie algebra of $SU(4)$, given by the following set of fifteen matrices:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_5 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_9 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_{10} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_{11} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \qquad \lambda_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix},$$

$$\lambda_{13} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \lambda_{14} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix},$$

$$\lambda_{15} = \tfrac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}.$$

The above generators of $SU(4)$ are traceless, Hermitian, and obey the extra relations:

$$\begin{aligned} [\lambda_i, \lambda_j] &= 2if_{ijk}\lambda_k \\ f_{ijk} &= \frac{1}{4i}\mathrm{Tr}\Big[[\lambda_i, \lambda_j] \cdot \lambda_k\Big]. \end{aligned}$$

The $SU(4)$ operators are given by:

$$\begin{aligned}
\hat{K}_1 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) \\
\hat{K}_2 &= \frac{1}{2i}(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1) \\
\hat{K}_3 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2) \\
\hat{K}_4 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_3 + \hat{a}_3^\dagger \hat{a}_1) \\
\hat{K}_5 &= \frac{1}{2i}(\hat{a}_1^\dagger \hat{a}_3 - \hat{a}_3^\dagger \hat{a}_1) \\
\hat{K}_6 &= \frac{1}{2}(\hat{a}_2^\dagger \hat{a}_3 + \hat{a}_3^\dagger \hat{a}_2) \\
\hat{K}_7 &= \frac{1}{2i}(\hat{a}_2^\dagger \hat{a}_3 - \hat{a}_3^\dagger \hat{a}_2) \\
\hat{K}_8 &= \frac{1}{2\sqrt{3}}(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 - 2\hat{a}_3^\dagger \hat{a}_3) \\
\hat{K}_9 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_4 + \hat{a}_4^\dagger \hat{a}_1) \\
\hat{K}_{10} &= \frac{1}{2i}(\hat{a}_1^\dagger \hat{a}_4 - \hat{a}_4^\dagger \hat{a}_1) \\
\hat{K}_{11} &= \frac{1}{2}(\hat{a}_2^\dagger \hat{a}_4 + \hat{a}_4^\dagger \hat{a}_2) \\
\hat{K}_{12} &= \frac{1}{2i}(\hat{a}_2^\dagger \hat{a}_4 - \hat{a}_4^\dagger \hat{a}_2) \\
\hat{K}_{13} &= \frac{1}{2}(\hat{a}_3^\dagger \hat{a}_4 + \hat{a}_4^\dagger \hat{a}_3) \\
\hat{K}_{14} &= \frac{1}{2i}(\hat{a}_3^\dagger \hat{a}_4 - \hat{a}_4^\dagger \hat{a}_3) \\
\hat{K}_{15} &= \frac{1}{2\sqrt{6}}(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 + \hat{a}_3^\dagger \hat{a}_3 - 3\hat{a}_4^\dagger \hat{a}_4) \\
\hat{K}_0 &= \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 + \hat{a}_3^\dagger \hat{a}_3),
\end{aligned}$$

from which we obtain the relations:

$$\begin{aligned}
\hat{a}_1^\dagger \hat{a}_1 &= \frac{1}{2}\hat{K}_0 + \hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15} \\
\hat{a}_2^\dagger \hat{a}_2 &= \frac{1}{2}\hat{K}_0 - \hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15} \\
\hat{a}_3^\dagger \hat{a}_3 &= \frac{1}{2}\hat{K}_0 - \frac{2}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15} \\
\hat{a}_4^\dagger \hat{a}_4 &= \frac{1}{2}\hat{K}_0 - \frac{3}{\sqrt{6}}\hat{K}_{15}.
\end{aligned}$$

In terms of the $\hat{K}$ operators, Eq. (5.15) becomes:

$$\begin{aligned}
\rho^{SE}(\tau) &= \frac{1}{Z} e^{-2i\omega\tau(g_{12}\hat{K}_1 + g_{23}\hat{K}_6 + g_{34}\hat{K}_{13})} \\
&\times\ e^{-\omega\theta_1\left(\frac{1}{2}\hat{K}_0 + \hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15}\right)} \times e^{-\omega\theta_2\left(\frac{3}{2}\hat{K}_0 - \hat{K}_3 - \frac{1}{\sqrt{3}}\hat{K}_8 - \frac{1}{\sqrt{6}}\hat{K}_{15}\right)} \\
&\times\ e^{+2i\omega\tau(g_{12}\hat{K}_1 + g_{23}\hat{K}_6 + g_{34}\hat{K}_{13})}. \qquad (5.16)
\end{aligned}$$

After some simplifying, Eq. (5.16) can be written as:

$$\begin{aligned}
\rho^{SE}(\tau) &= \frac{1}{Z} e^{-\frac{1}{2}\omega\hat{K}_0(\theta_1 + 3\theta_2)} \times e^{-2i\omega\tau(g_{12}\hat{K}_1 + g_{23}\hat{K}_6 + g_{34}\hat{K}_{13})} \\
&\times\ e^{-\omega(\theta_1 - \theta_2)(\hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15})} \times e^{+2i\omega\tau(g_{12}\hat{K}_1 + g_{23}\hat{K}_6 + g_{34}\hat{K}_{13})}.
\end{aligned}$$

The matrix elements of the reduced, time-evolved system density matrix after one characteristic time interval τ has passed are given by:

$$\begin{aligned}
\langle n_1' | \rho^S(\tau) | n_1 \rangle &= \delta_{n_1', n_1} \sum_{n_2, n_3, n_4} \langle n_1', n_2, n_3, n_4 | \rho^{SE}(\tau) | n_1, n_2, n_3, n_4 \rangle \\
&= \delta_{n_1', n_1} \frac{1}{Z} \sum_{n_2, n_3, n_4} \langle n_1', n_2, n_3, n_4 | e^{-\alpha_{04}\hat{K}_0} e^{-2i\omega\tau(g_{12}\hat{K}_1 + g_{23}\hat{K}_6 + g_{34}\hat{K}_{13})} \\
&\times\ e^{-\omega(\theta_1 - \theta_2)(\hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15})} e^{+2i\omega\tau(g_{12}\hat{K}_1 + g_{23}\hat{K}_6 + g_{34}\hat{K}_{13})} | n_1, n_2, n_3, n_4 \rangle,
\end{aligned}$$

or:

$$\begin{aligned}\langle n_1'|\rho^S(\tau)|n_1\rangle &= \delta_{n_1',n_1}\frac{1}{Z}\sum_{n_2,n_3,n_4} e^{-\alpha_{04}\frac{N}{2}}\langle n_1',n_2,n_3,n_4|e^{-2i\omega\tau\hat{H}_{int}^{SU(4)}} \\ &\times\ e^{-\omega(\theta_1-\theta_2)(\hat{K}_3+\frac{1}{\sqrt{3}}\hat{K}_8+\frac{1}{\sqrt{6}}\hat{K}_{15})}e^{+2i\omega\tau\hat{H}_{int}^{SU(4)}}|n_1,n_2,n_3,n_4\rangle,\end{aligned} \tag{5.17}$$

where:

$$\alpha_{04}=\frac{2}{4}\omega(\theta_1+3\theta_2).$$

To solve Eq. (5.17), we need to calculate the action of $\hat{H}_{int}^{SU(4)}$ on the state $|n_1,n_2,n_3,n_4\rangle$, or:

$$e^{+2i\omega\tau\hat{H}_{int}}|n_1,n_2,n_3,n_2\rangle = e^{+2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6+g_{34}\hat{K}_{13})} = \hat{\Re}^{SU(4)}|n_1,n_2,n_3,n_4\rangle. \tag{5.18}$$

This can be done by following a procedure similar to that presented in Section 5.1 for the $SU(3)$ case. Once Eq. (5.18) is solved, the reduced matrix elements for the system become:

$$\langle n_1'|\rho^S(\tau)|n_1\rangle = \frac{\delta_{n_1',n_1}}{Z}\sum_{n_2,n_3,n_4} e^{-\alpha_{04}\frac{N}{2}}e^{-\frac{\omega}{4}(\theta_1-\theta_2)(3n_1-n_2-n_3-n_4)}|f(n_1,n_2,n_3,n_4)|^2, \tag{5.19}$$

where $f(n_1,n_2,n_3,n_4)$ is the eigenvalue of $\hat{\Re}^{SU(4)}$.

5.2.2 The case of $SU(5)$

The free and interaction Hamiltonians for the case of $SU(5)$ are given by:

$$\begin{aligned}
\hat{H}_{free} &= \omega \sum_{i=1}^{5} \hat{a}_i^\dagger \hat{a}_i \\
\hat{H}_{int}^{SU(5)} &= \omega \sum_{i=1}^{4} g_{i,i+1}(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i),
\end{aligned}$$

and the time-evolved composite density matrix $\rho^{SE}(\tau)$ is:

$$\begin{aligned}
\rho^{SE}(\tau) &= \frac{1}{Z} e^{-i\omega\tau \Big[\sum_{i=1}^{5} \hat{a}_i^\dagger \hat{a}_i + \sum_{i=1}^{4} g_{i,i+1}(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i) \Big]} \\
&\times \; e^{-\omega \Big[\theta_1 \hat{a}_1^\dagger \hat{a}_1 + \theta_2 \sum_{i=2}^{5} \hat{a}_i^\dagger \hat{a}_i \Big]} \\
&\times \; e^{+i\omega\tau \Big[\sum_{i=1}^{5} \hat{a}_i^\dagger \hat{a}_i + \sum_{i=1}^{4} g_{i,i+1}(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i) \Big]}, \qquad (5.20)
\end{aligned}$$

where $Z = Z_1 Z_2 Z_3 Z_4 Z_5$. The Gell-Mann type basis for the Lie algebra of $SU(5)$ is given by a set of twenty-four matrices. The first fifteen are the same as those for the $SU(4)$ case (with the fifth row and column all zeroes), and the remaining nine are:

$$\lambda_{16} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_{17} = \begin{pmatrix} 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_{18} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \qquad \lambda_{19} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_{20} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}, \qquad \lambda_{21} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 \end{pmatrix},$$

$$\lambda_{22} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \lambda_{23} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & i & 0 \end{pmatrix},$$

$$\lambda_{24} = \tfrac{1}{\sqrt{10}} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -4 \end{pmatrix}.$$

The corresponding $SU(5)$ operators are:

$$\begin{aligned}
\hat{K}_{16} &= \frac{1}{2}(\hat{a}_1^\dagger\hat{a}_5 + \hat{a}_5^\dagger\hat{a}_1) \\
\hat{K}_{17} &= \frac{1}{2i}(\hat{a}_1^\dagger\hat{a}_5 - \hat{a}_5^\dagger\hat{a}_1) \\
\hat{K}_{18} &= \frac{1}{2}(\hat{a}_2^\dagger\hat{a}_5 - \hat{a}_5^\dagger\hat{a}_2) \\
\hat{K}_{19} &= \frac{1}{2}(\hat{a}_2^\dagger\hat{a}_5 + \hat{a}_5^\dagger\hat{a}_2) \\
\hat{K}_{20} &= \frac{1}{2i}(\hat{a}_3^\dagger\hat{a}_5 - \hat{a}_5^\dagger\hat{a}_3) \\
\hat{K}_{21} &= \frac{1}{2}(\hat{a}_3^\dagger\hat{a}_5 + \hat{a}_5^\dagger\hat{a}_3) \\
\hat{K}_{22} &= \frac{1}{2i}(\hat{a}_4^\dagger\hat{a}_5 - \hat{a}_5^\dagger\hat{a}_4) \\
\hat{K}_{23} &= \frac{1}{2i}(\hat{a}_4^\dagger\hat{a}_5 + \hat{a}_5^\dagger\hat{a}_4) \\
\hat{K}_{24} &= \frac{1}{2\sqrt{10}}(\hat{a}_1^\dagger\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_2 + \hat{a}_3^\dagger\hat{a}_3 + \hat{a}_4^\dagger\hat{a}_4 - 4\hat{a}_5^\dagger\hat{a}_5),
\end{aligned}$$

from which we obtain the relations:

$$\begin{aligned}
\hat{a}_1^\dagger\hat{a}_1 &= \frac{6}{15}\hat{K}_0 + \hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15} + \frac{1}{\sqrt{10}}\hat{K}_{24} \\
\hat{a}_2^\dagger\hat{a}_2 &= \frac{6}{15}\hat{K}_0 - \hat{K}_3 + \frac{1}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15} + \frac{1}{\sqrt{10}}\hat{K}_{24} \\
\hat{a}_3^\dagger\hat{a}_3 &= \frac{6}{15}\hat{K}_0 - \frac{2}{\sqrt{3}}\hat{K}_8 + \frac{1}{\sqrt{6}}\hat{K}_{15} + \frac{1}{\sqrt{10}}\hat{K}_{24} \\
\hat{a}_4^\dagger\hat{a}_4 &= \frac{2}{5}\hat{K}_0 - \frac{1}{2\sqrt{6}}\hat{K}_{15} + \frac{1}{\sqrt{10}}\hat{K}_{24} \\
\hat{a}_5^\dagger\hat{a}_5 &= \frac{2}{5}\hat{K}_0 - \frac{4}{\sqrt{10}}\hat{K}_{24},
\end{aligned}$$

with:

$$\hat{K}_0 = \frac{1}{2}(\hat{a}_1^\dagger\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_2 + \hat{a}_3^\dagger\hat{a}_3 + \hat{a}_4^\dagger\hat{a}_4 + \hat{a}_5^\dagger\hat{a}_5).$$

In terms of the above $\hat{K}$ operators, Eq. (5.20) becomes:

$$\begin{aligned}\rho^{SE}(\tau) &= \frac{1}{Z}e^{-\frac{2}{5}\omega\hat{K}_0(\theta_1+4\theta_2)} \times e^{-2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6+g_{34}\hat{K}_{13}+g_{45}\hat{K}_{22})} \\ &\times \; e^{-\omega(\theta_1-\theta_2)(\hat{K}_3+\frac{1}{\sqrt{3}}\hat{K}_8+\frac{1}{\sqrt{6}}\hat{K}_{15}+\frac{1}{\sqrt{10}}\hat{K}_{24})}e^{+2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6+g_{34}\hat{K}_{13}+g_{45}\hat{K}_{22})}.\end{aligned}$$

The matrix elements of the time-evolved reduced density matrix are given by:

$$\begin{aligned}\langle n_1'|\rho^S(\tau)|n_1\rangle &= \frac{\delta_{n_1',n_1}}{Z}\sum_{n_2,n_3,n_4,n_5} e^{-\alpha_{05}\frac{N}{2}}\langle n_1',n_2,n_3,n_4,n_5|e^{-2i\omega\tau\hat{H}_{int}^{SU(5)}} \\ &\times \; e^{-\omega(\theta_1-\theta_2)(\hat{K}_3+\frac{1}{\sqrt{3}}\hat{K}_8+\frac{1}{\sqrt{6}}\hat{K}_{15}+\frac{1}{\sqrt{10}}\hat{K}_{24})}e^{+2i\omega\tau\hat{H}_{int}^{SU(5)}}|n_1,n_2,n_3,n_4,n_5\rangle, \end{aligned} \tag{5.21}$$

where:

$$\alpha_{05} = \frac{2}{5}\omega(\theta_1+4\theta_2).$$

Once again, the solution of Eq. (5.21) depends on calculating the action of $\hat{H}_{int}^{SU(5)}$ on the state $|n_1,n_2,n_3,n_4,n_5\rangle$, or:

$$e^{+2i\omega\tau(g_{12}\hat{K}_1+g_{23}\hat{K}_6+g_{34}\hat{K}_{13}+g_{45}K_{22})} = \hat{\Re}^{SU(5)}|n_1,n_2,n_3,n_4,n_5\rangle. \tag{5.22}$$

Just like in the previous cases, once Eq. (5.22) is solved, the reduced matrix elements for the system become:

$$\begin{aligned}\langle n_1'|\rho^S(\tau)|n_1\rangle &= \frac{\delta_{n_1',n_1}}{Z}\sum_{n_2,n_3,n_4,n_5} e^{-\alpha_{05}\frac{N}{2}}e^{-\frac{\omega}{5}(\theta_1-\theta_2)(4n_1-n_2-n_3-n_4-n_5)} \\ &\times \; |f(n_1,n_2,n_3,n_4,n_5)|^2,\end{aligned} \tag{5.23}$$

where $f(n_1,n_2,n_3,n_4,n_5)$ is the eigenvalue of $\hat{\Re}^{SU(5)}$.

5.3 The generalization to $SU(N)$

We are now in a position to generalize our results to the case of an arbitrary number of interacting oscillators. The algebra of $SU(N)$ can be used to describe the case in which the physical system of interest is a single harmonic oscillator and the environment with which this system is in contact is a chain composed of $N-1$ harmonic oscillators. The interaction Hamiltonian for an arbitrary $SU(N)$ is of the form:

$$\hat{H}^{SU(N)}_{int} = \omega \sum_{i=1}^{N-1} g_{i,i+1}(\hat{a}^{\dagger}_i \hat{a}_{i+1} + \hat{a}^{\dagger}_{i+1}\hat{a}_i),$$

and the initial composite density matrix of such a system is given by:

$$\begin{aligned} \rho^{SE}(\tau) &= \frac{1}{Z} e^{-i\omega\tau\Big[\sum_{i=1}^{N} \hat{a}^{\dagger}_i \hat{a}_i + \sum_{i=1}^{N-1} g_{i,i+1}(\hat{a}^{\dagger}_i \hat{a}_{i+1} + \hat{a}^{\dagger}_{i+1}\hat{a}_i)\Big]} \\ &\times\ e^{-\omega\Big[\theta_1 \hat{a}^{\dagger}_1 \hat{a}_1 + \theta_2 \sum_{i=2}^{N} \hat{a}^{\dagger}_i \hat{a}_i\Big]} \\ &\times\ e^{+i\omega\tau\Big[\sum_{i=1}^{N} \hat{a}^{\dagger}_i \hat{a}_i + \sum_{i=1}^{N-1} g_{i,i+1}(\hat{a}^{\dagger}_i \hat{a}_{i+1} + \hat{a}^{\dagger}_{i+1}\hat{a}_i)\Big]}, \end{aligned}$$

and $Z = Z_1 Z_2 \cdots Z_N$.

To obtain the generators for an arbitrary $SU(N)$, we define two $N \times N$ matrices for every $i, j = 1, 2, 3, \cdots, N$ [17, 20], such that:

$$[\lambda^{\{1\}}(i,j)]_{\mu\nu} = \delta_{j\mu}\delta_{i\nu} + \delta_{j\nu}\delta_{i\mu},$$

and:

$$[\lambda^{\{2\}}(i,j)]_{\mu\nu} = -i(\delta_{i\mu}\delta_{j\nu} - \delta_{i\nu}\delta_{j\mu}).$$

The above forms $N(N+1)$ linearly independent matrices. We can then construct a further $N-1$ matrices according to:

$$\lambda_{n^2-1} = \begin{pmatrix} (1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1)_{n-1} & 0 & \cdots & 0 \\ 0 & 0 & 0 & -(n-1) & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}_{N\times N},$$

for $n = 2, 3, \cdots, N$. From these generators, N^2-1 operators can be defined.

Once the $SU(N)$ operators are constructed, the matrix elements of the reduced density matrix $\rho^S(\tau)$ after one characteristic time interval has passed will be given by:

$$\begin{aligned} \langle n_1'|\rho^S(\tau)|n_1\rangle &= \frac{\delta_{n_1',n_1}}{Z} \sum_{n_2,n_3,\cdots,n_N} e^{-\alpha_{0N}\frac{N}{2}} e^{-\frac{\omega}{N}(\theta_1-\theta_2)\Big[(N-1)n_1-n_2-\cdots-n_N\Big]} \\ &\times \; |f(n_1,n_2,\cdots,n_N)|^2, \end{aligned} \tag{5.24}$$

with:

$$\alpha_{0N} = \frac{2}{N}\omega\Big[\theta_1 + (N-1)\theta_2\Big].$$

Equation (5.24) was constructed by comparing Eqs. (5.12), (5.19), and (5.23). The difficulty in calculating $\hat{\Re}^{SU(N)}|n_1, n_2, \cdots, n_N\rangle = f(n_1, n_2, \cdots, n_N)|n_1, n_2, \cdots, n_N\rangle$ increases more and more as N becomes larger. We have shown that even with N as small as 3, this calculation was significantly tedious.

Following the discussion of the $SU(2)$ and $SU(3)$ cases, we can expect that the initial Maxwell-Boltzmann distribution of our physical system will be replaced by a second Maxwell-Boltzmann distribution at temperature $T_1(\tau)$ after one characteristic interval τ has passed. In theory, one should be able to calculate $\langle n_1'|\rho^S(2\tau)|n_1\rangle$, $\cdots$, $\langle n_1'|\rho^S(n\tau)|n_1\rangle$ numerically or analytically for an arbitrary number N of interacting harmonic oscillators. Even though Eqs. (5.12), (5.19), and (5.23) have not been solved explicitly, the analysis presented for the $SU(2)$ and $SU(3)$ cases allows us to conclude that the physical system of interest will always reach a new steady $\rho^S(n\tau)$ such that $\theta_1(\infty) = \theta_2(0)$ when the frequency of the system is the same as that of the environment, and such that $\omega_1\theta_1(\infty) = \omega_2\theta_2(0)$ when the frequencies of the system and the environment are not equal.

Chapter 6

A transition to quantum optics

Chapter 5 completes our study of the relaxation of open quantum mechanical harmonic oscillator systems and along with it the first part of this dissertation. We now make a transition from the quantum mechanical analysis of open systems to the classical analysis of electromagnetic wave propagation and optical phenomena inside left-handed materials. Even though the study of these two problems is complete within each topic's own context, we present this chapter as a link between the quantum mechanical analysis of the harmonic oscillator and that of the electromagnetic field. The connection between the two, lies in the fact that field quantization is based on recognizing that the electromagnetic field is equivalent to an infinite set of harmonic oscillators.

Historically, any attempts in explaining phenomena such as the interaction of light with matter, electron diffraction, or atomic spectra using classical description failed. It was soon realized that only a quantum mechanical approach could be successful. In making the transition from classical to quantum theory, classical variables are replaced by operators and the states of the system are replaced by state vectors. Following this general procedure, all physical observables appearing in nature (including field variables describing wave phenomena) must be accounted for by operators.

We have already employed the quantum mechanical description of a harmonic oscillator in the calculations of Chapter 4, without formally deriving it. In Section 6.1, we present a formal derivation of the quantum theory of the harmonic oscillator, before we proceed to the quantization of the electromagnetic field in Section 6.2.

6.1 The harmonic oscillator

Consider a classical harmonic oscillator with coordinate q, conjugate momentum $p = m\dot{q}$, and mass m. The Hamiltonian of this harmonic oscillator is given by:

$$H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}. \tag{6.1}$$

The canonical equations of motion give for this Hamiltonian:

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m} \\ \dot{p} &= -\frac{\partial H}{\partial q} = -m\omega^2 q, \end{aligned}$$

in agreement with Newton's Laws of motion.

To make the transformation from the classical to the quantum theory, we need to replace q, p, and H with the analogous operators. The Hamiltonian (6.1) becomes:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{q}^2}{2}, \tag{6.2}$$

with $\hat{q}$ and $\hat{p}$ satisfying the commutation relation:

$$[\hat{q}, \hat{p}] = i.$$

The operators $\hat{q}$ and $\hat{p}$ are Hermitian and unbounded.

6.1.1 Second quantization: creation and annihilation operators

We can now make a change of basis by defining the two non-Hermitian operators:

$$\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2m\omega}}(m\omega\hat{q} + i\hat{p}) & (6.3) \\ \hat{a}^\dagger &= \frac{1}{\sqrt{2m\omega}}(m\omega\hat{q} - i\hat{p}). & (6.4) \end{aligned}$$

These are the well-known lowering (or annihilation) and raising (or creation) operators, respectively. In terms of these new operators, $\hat{q}$ and $\hat{p}$ can be written as:

$$\begin{aligned} \hat{q} &= \sqrt{\frac{1}{2m\omega}}(\hat{a} + \hat{a}^\dagger) & (6.5) \\ \hat{p} &= i\sqrt{\frac{m\omega}{2}}(\hat{a}^\dagger - \hat{a}). & (6.6) \end{aligned}$$

It can be shown that:

$$[\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0,$$

and

$$[\hat{a}, \hat{a}^\dagger] = 1.$$

In terms of these new operators, the Hamiltonian (6.2) becomes:

$$\hat{H} = \omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{6.7}$$

and its eigenstates are states of definite energy, satisfying:

$$\hat{H}|n\rangle = \omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|n\rangle = E_n|n\rangle, \tag{6.8}$$

where E_n is the energy of state $|n\rangle$. The states $|n\rangle$ are known as Fock or number states. We can also define the Hermitian operator known as the number operator

$\hat{N} = \hat{a}^\dagger \hat{a}$, which leads us to an important relation between $\hat{N}$ and $\hat{H}$:

$$\hat{H} = \omega \left(\hat{N} + \frac{1}{2} \right). \tag{6.9}$$

Because $\hat{H}$ is just a linear function of $\hat{N}$, $\hat{N}$ and $\hat{H}$ can be simultaneously diagonalized. If we denote the eigenvalue of $\hat{N}$ by n, we obtain the eigenvalue equation:

$$\hat{N}|n\rangle = n|n\rangle. \tag{6.10}$$

Combining Eqs. (6.8), (6.9), and (6.10) gives the energy eigenvalues of the oscillator:

$$E_n = \left(n + \frac{1}{2} \right) \omega.$$

We can appreciate the physical significance of $\hat{a}$, $\hat{a}^\dagger$, and $\hat{N}$ by first noting that:

$$[\hat{N}, \hat{a}] = [\hat{a}^\dagger \hat{a}, \hat{a}] = -\hat{a},$$

and

$$[\hat{N}, \hat{a}^\dagger] = [\hat{a}^\dagger \hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger.$$

This leads to the important relations:

$$\begin{aligned} \hat{N}\hat{a}^\dagger|n\rangle &= (n+1)\hat{a}^\dagger|n\rangle & (6.11) \\ \hat{N}\hat{a}|n\rangle &= (n-1)\hat{a}|n\rangle. & (6.12) \end{aligned}$$

Equations (6.11) and (6.12) imply that both $\hat{a}^\dagger|n\rangle$ and $\hat{a}|n\rangle$ are eigenkets of $\hat{N}$ with eigenvalues increased and decreased by one, respectively. The increase of n by one amounts to the creation of a single quantum unit of energy and, in analogy, the decrease of n by one corresponds to an annihilation of a single quantum unit of energy. This is precisely how the operators get their names.

Further, Eq. (6.12) implies that:

$$\hat{a}|n\rangle = c|n-1\rangle,$$

where c is a numerical constant that can be determined from the requirement that both $|n\rangle$ and $|n-1\rangle$ be normalized. This can be done by noting that:

$$\langle n|\hat{a}^\dagger \hat{a}|n\rangle = |c|^2,$$

such that $n = |c|^2$. By taking c to be real and positive by convention, it can be shown that:

$$\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}|n-1\rangle \qquad (6.13) \\ \hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle. \qquad (6.14) \end{aligned}$$

If the annihilation operator $\hat{a}$ is repeatedly applied to both sides of Eq. (6.13), a sequence of smaller and smaller values of n is obtained. This sequence will eventually terminate as long as we start with a positive integer n. The positivity requirement for the norm of $\hat{a}|n\rangle$ leads to the conclusion that n can never be negative and that the sequence terminates with $n = 0$. In turn, this implies that the ground state of the harmonic oscillator is $|0\rangle$, with ground energy $E_0 = (1/2)\omega$.

The simultaneous eigenkets of $\hat{H}$ and $\hat{N}$ can be obtained by repeated application of the creation operator $\hat{a}^\dagger$ to the ground state $|0\rangle$. They are found to be:

$$|n\rangle = \left[\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\right]\Big|0\Big\rangle,$$

with energy eigenvalues given by:

$$E_n = \left(n + \frac{1}{2}\right)\omega,$$

and $n = 0, 1, 2, 3, ...$

6.2 The electromagnetic field

We are now ready to quantize the electromagnetic field to show that it is equivalent to an infinite set of harmonic oscillators. Each harmonic oscillator is quantized using the canonical procedure as shown above. The result is a representation of the field as a sum over modes at frequencies ω_i, with each of these frequencies having a definite number n_i of quanta, or excitations. Just as in the case of the quantum harmonic oscillator, each excitation of the field contributes an energy ω_i, such that the total energy of the field is expressed as:

$$E = \sum_i \omega_i \left(n_i + \frac{1}{2} \right).$$

6.2.1 Normal mode expansion

In order to quantize the electromagnetic field by the procedure developed in Section 6.1, a normal mode expansion for the field must be introduced. To arrive at a discrete set of modes, we define an artificial "quantization volume" V. For simplicity, we consider the "free field" case, in which there are no particles, no charges, and no current, so that the only source of the electric field is the change in the magnetic field, and vice versa. We specifically consider a plane optical wave propagating in the z direction between two plane x-y surfaces of perfect conductivity separated by a length L. This set-up is nothing more than a plane-wave resonator of length L and volume $V = LA$, where A is the cross-sectional area of the end surfaces.

In source-free space, Maxwell's equations are:

$$\begin{aligned}
\nabla \times \mathbf{E}(\mathbf{r},t) &= -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t) && (6.15)\\
\nabla \times \mathbf{B}(\mathbf{r},t) &= \epsilon_0\mu_0\frac{\partial}{\partial t}\mathbf{E}(\mathbf{r},t) && (6.16)\\
\nabla \cdot \mathbf{E}(\mathbf{r},t) &= 0 && (6.17)\\
\nabla \cdot \mathbf{B}(\mathbf{r},t) &= 0 && (6.18)
\end{aligned}$$

Besides satisfying Maxwell's equations, the electric field $\mathbf{E}(\mathbf{r},t)$ must also satisfy the boundary conditions $\mathbf{E}(z=0,t) = \mathbf{E}(z=L,t) = 0$. The fields can be expanded as:

$$\begin{aligned}
\mathbf{E}(\mathbf{r},t) &= -\sqrt{\frac{1}{\epsilon_0}}\sum_{l,\sigma} p_{l,\sigma}(t)\mathbf{E}_{l,\sigma}(z) && (6.19)\\
\mathbf{B}(\mathbf{r},t) &= \sqrt{\mu_0}\sum_{l,\sigma} \omega_l q_{l,\sigma}(t)\mathbf{B}_{l,\sigma}(z). && (6.20)
\end{aligned}$$

Here, l is a positive integer, $c = 1/\epsilon_0\mu_0$ is the speed of light, and μ_0 and ϵ_0 are the magnetic permeability and electric permittivity of vacuum, respectively. Finally, $\omega_l = k_l c$ is the frequency of the l^{th} resonator mode. The field distributions of the l^{th} mode with the electric field polarized along the unit vector pointing along the σ direction, $\mathbf{e}_\sigma$, are given by:

$$\begin{aligned}
\mathbf{E}_{l,\sigma}(z) &= \mathbf{e}_\sigma\sqrt{\frac{2}{V}}\sin k_l z && (6.21)\\
\mathbf{B}_{l,\sigma}(z) &= \mathbf{e}_\sigma \times \mathbf{e}_z\sqrt{\frac{2}{V}}\cos k_l z, && (6.22)
\end{aligned}$$

where:

$$k_l = \frac{2\pi}{L}l,$$

and $\sigma = x, y$. With the proper normalization, the modes are orthogonal, obeying:

$$\int_V \mathbf{E}_{l,\sigma} \cdot \mathbf{E}_{m,\gamma} d^3r = \delta_{l.m}\delta_{\sigma,\gamma} \tag{6.23}$$

$$\int_V \mathbf{B}_{l,\sigma} \cdot \mathbf{B}_{m,\gamma} d^3r = \delta_{l.m}\delta_{\sigma,\gamma}. \tag{6.24}$$

After substituting Eqs. (6.19) - (6.22) into Maxwell's Eqs. (6.15) and (6.16), we obtain:

$$p_{l,\sigma} = \frac{dq_{l,\sigma}}{dt} \tag{6.25}$$

$$\omega_l^2 q_{l,\sigma} = -\frac{dp_{l,\sigma}}{dt}, \tag{6.26}$$

which in turn lead to:

$$\frac{d^2 q_{l,\sigma}}{dt^2} + \omega_l^2 q_{l,\sigma} = 0. \tag{6.27}$$

Equation (6.27) is precisely that of simple harmonic motion, with ω_l being the oscillation frequency of the l^{th} mode. This is now starting to look exactly like we wished it would.

The next step is to calculate the energy stored in the electromagnetic field. This is given by:

$$H_{field} = \frac{1}{2}\int_V \left(\epsilon_0 \mathbf{E}^2 + \frac{1}{\mu_0}\mathbf{B}^2\right) d^3r, \tag{6.28}$$

for all modes put together. In terms of the dynamical variables $q_{l,\sigma}(t)$ and $p_{l,\sigma}(t)$, Eq. (6.28) can be written as:

$$H_{field} = \frac{1}{2}\sum_{l,\sigma}(p_{l,\sigma}^2 + \omega_l^2 q_{l,\sigma}^2). \tag{6.29}$$

Equation (6.29) was obtained by using the normalization conditions (6.23) and (6.24), and by substituting Eqs. (6.19) and (6.20) into (6.28). Comparison of Eq. (6.29) with Eq. (6.1) suggests that mathematically, the electromagnetic field in the resonator behaves just like an ensemble of independent harmonic oscillators. The canonical variables $q_{l,\sigma}$ and $p_{l,\sigma}$ constitute the canonically conjugate position and momentum variables q and p. This last statement can be verified by writing down Hamilton's equations of motion:

$$\begin{aligned} \dot{q}_{l,\sigma} &= \frac{\partial H}{\partial p_{l,\sigma}} = p_{l,\sigma} && (6.30) \\ \dot{p}_{l,\sigma} &= -\frac{\partial H}{\partial q_{l,\sigma}} = -\omega_l^2 q_{l,\sigma}. && (6.31) \end{aligned}$$

Equations (6.30) and (6.31) are the same as Eqs. (6.25) and (6.26) obtained from Maxwell's equations.

6.2.2 Quantization of the electromagnetic field

Now that we have expanded the electromagnetic field in normal modes, it's quantization is straight-forward. It can be implemented simply by following the quantization procedure for the harmonic oscillator. Once again, we define the creation and annihilation operators $\hat{a}_{l,\sigma}$ and $\hat{a}^{\dagger}_{l,\sigma}$, analogous to Eqs. (6.3) and (6.4):

$$\begin{aligned} \hat{a}_{l,\sigma} &= \frac{1}{\sqrt{2\omega_l}}(\omega_l \hat{q}_{l,\sigma} + i\hat{p}_{l,\sigma}) && (6.32) \\ \hat{a}^{\dagger}_{l,\sigma} &= \frac{1}{\sqrt{2\omega_l}}(\omega_l \hat{q}_{l,\sigma} - i\hat{p}_{l,\sigma}). && (6.33) \end{aligned}$$

In analogy to the harmonic oscillator case, the operators (6.32) and (6.33) obey the commutation relations:

$$[\hat{a}_{l,\sigma}, \hat{a}_{m,\gamma}] = [\hat{a}^{\dagger}_{l,\sigma}, \hat{a}^{\dagger}_{m,\gamma}] = 0$$

$$[\hat{a}_{l,\sigma}, \hat{a}^{\dagger}_{m,\gamma}] = \delta_{l,m}\delta_{\sigma,\gamma}.$$

Following Eqs. (6.5) and (6.6), we can write the position and momentum operators as:

$$\hat{q}_{l,\sigma} = \sqrt{\frac{1}{2\omega_l}}(\hat{a}_{l,\sigma} + \hat{a}^{\dagger}_{l,\sigma}) \tag{6.34}$$

$$\hat{p}_{l,\sigma} = i\sqrt{\frac{\omega_l}{2}}(\hat{a}^{\dagger}_{l,\sigma} - \hat{a}_{l,\sigma}). \tag{6.35}$$

We can now write the operator expressions for the electric and magnetic fields of the resonator by substituting Eqs. (6.34) and (6.35) into Eqs. (6.19) and (6.20):

$$\begin{aligned}
\hat{\mathbf{E}} &= -i\sum_{l,\sigma}\mathbf{e}_{\sigma}\sqrt{\frac{\omega_l}{\epsilon_0 V}}(\hat{a}^{\dagger}_{l,\sigma} - \hat{a}_{l,\sigma})\sin k_l z \\
\hat{\mathbf{B}} &= \sum_{l,\sigma}(\mathbf{e}_{\sigma} \times \mathbf{e}_z)k_l\sqrt{\frac{1}{\epsilon_0 V\omega_l}}(\hat{a}^{\dagger}_{l,\sigma} + \hat{a}_{l,\sigma})\cos k_l z.
\end{aligned}$$

The Hamiltonian of the field can be written in terms of the raising and lowering operators, taking a form analogous to Eq. (6.7):

$$\hat{H}_{field} = \sum_{l,\sigma}\omega_l\left(\hat{a}^{\dagger}_{l,\sigma}\hat{a}_{l,\sigma} + \frac{1}{2}\right).$$

The Hilbert space describing the quantized electromagnetic field is a Fock space. A state with n photons in the l^{th} mode polarized in the σ direction is given by acting n times with the creation operator $\hat{a}^{\dagger}_{l,\sigma}$ on the vacuum state $|0\rangle$, and normalizing:

$$|n_{l,\sigma}\rangle = \frac{(\hat{a}_{l\sigma})^n}{\sqrt{n!}}|0\rangle.$$

Any state will be a superposition of such states for all modes.

Chapter 7

Wave propagation in left-handed materials

When neutral matter is placed inside an electric field, it becomes *polarized.* This polarization comes about because the electric field induces electric dipoles which align in the direction of the field. The polarization of a medium is proportional to the field such that:

$$\mathbf{P} = \epsilon_0 \chi_e \mathbf{E},$$

where χ_e is the electric susceptibility of the medium and ϵ_0 is the electric permittivity of free space.

Similarly, matter becomes *magnetized* when placed inside a magnetic field. The magnetic dipoles align parallel (for paramagnets) or antiparallel (for diamagnets) to the direction of the field. The magnetization of the medium is analogous to the polarization and is proportional to the magnetic field:

$$\mathbf{M} = \frac{1}{\mu_0} \chi_m \mathbf{B},$$

where χ_m is the magnetic susceptibility of the medium and μ_0 is the permeability of free space.

For *linear* media, we define:

$$\begin{aligned}\mathbf{D} &\equiv \epsilon_0\mathbf{E}+\mathbf{P}=\epsilon\mathbf{E}\\ \mathbf{H} &\equiv \frac{1}{\mu_0}\mathbf{B}-\mathbf{M}=\frac{1}{\mu}\mathbf{B},\end{aligned}$$

where:

$$\begin{aligned}\epsilon &= \epsilon_0(1+\chi_e)\\ \mu &= \mu_0(1+\chi_m).\end{aligned}$$

The parameters ϵ and μ are known as the electric permittivity and magnetic permeability of the medium, respectively. Together, they describe how a medium responds when placed in an electromagnetic field.

The dispersion relation satisfied by an electromagnetic wave inside an isotropic medium is given by:

$$k^2=\frac{\omega^2 n^2}{c^2}, \tag{7.1}$$

where k is the wavenumber, c is the speed of the wave in vacuum, and n is the refractive index of the medium. We also have:

$$n^2\equiv\frac{\epsilon\mu}{\epsilon_0\mu_0},$$

or:

$$n=\pm\sqrt{\frac{\epsilon\mu}{\epsilon_0\mu_0}}. \tag{7.2}$$

Materials can be classified in terms of the sign of their electric permittivity and magnetic permeability. For materials found in nature, the positive sign of the square root in Eq. (7.2) applies. Almost all materials encountered in optics, such as glass or water, have positive values for both ϵ and μ. However, many metals (such as silver and gold), have negative ϵ at visible wavelengths. Materials having either (but not both) ϵ or μ negative are opaque to electromagnetic radiation (for example surface plasmons), since n becomes imaginary. To have n real, we need to look at materials with the same sign of ϵ and μ simultaneously. However, to this date, materials with both ϵ and μ negative for long wavelengths have not been found in nature.

The theoretical implications of materials with simultaneously negative permeability and permittivity were first studied by Victor Veselago, a Russian physicist, in 1968 [77]. Veselago suggested that the electromagnetic properties of such materials would exhibit interesting phenomena, without violating any fundamental physical laws. He also claimed that such materials would be characterized by a negative index of refraction, and would have unique properties such as a reversed Doppler effect, Cherenkov radiation, and even Snell's Law. Since then, a great deal of interest has been paid to these theories [49, 68, 71, 72].

From Eqs. (7.1) and (7.2), it is clear that a simultaneous change of the signs of ϵ and μ does not affect the equations. Substances with simultaneously negative ϵ and μ still satisfy the dispersion relation. To see how the properties of such a material would change, Veselago looked at Maxwell's equations in free space:

$$\begin{aligned}
\nabla \times \mathbf{E} &= -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \times \mathbf{H} &= \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \cdot \mathbf{D} &= 0,
\end{aligned}$$

where $\mathbf{D} = \epsilon\mathbf{E}$ and $\mathbf{H} = \mathbf{B}/\mu$. For a plane monochromatic wave in which all quantities are proportional to $e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$, the curl equations above take the form:

$$\begin{aligned}\mathbf{k}\times\mathbf{E} &= \frac{\omega}{c}\mu\mathbf{H}\\ \mathbf{k}\times\mathbf{H} &= -\frac{\omega}{c}\epsilon\mathbf{E}.\end{aligned}$$

For $\epsilon > 0$ and $\mu > 0$, $\mathbf{E}$, $\mathbf{H}$, and $\mathbf{k}$ form a right-handed triplet of vectors, while for $\epsilon < 0$ and $\mu < 0$, they form a left-handed triplet of vectors. For this reason, materials like these have since then been given the name "left-handed materials".

Even though materials with ϵ and μ negative simultaneously are not known to exist in nature, it has been recently suggested that such materials can be fabricated over a finite frequency band by specific electromagnetic design. Such a one-dimensional structure was introduced by Smith *et al.* in [67]. Subsequently, an extension to two dimensions was presented by Shelby *et al.*, and such an artificial composite was predicted to have an isotropic, negative index of refraction in two dimensions [64]. Recent technological advances have made this goal realizable. In fact, experimental scattering data at microwave frequencies on a structured material that exhibits a frequency band where the effective index of refraction is negative, directly confirms Veselago's predictions [65].

To produce a negative electric permittivity in a particular frequency region, wire elements were used [47], while at the same time, non-magnetic thin sheets of metal were utilized to create a negative magnetic permeability in an overlapping frequency region [48]. Both ϵ and μ rely on a resonant response and have the resonant form [65]:

$$\begin{aligned}\frac{\mu(\omega)}{\mu_0} &= 1-\frac{\omega_{mp}^2-\omega_{mo}^2}{\omega^2-\omega_{mo}^2+i\gamma\omega}\\ \frac{\epsilon(\omega)}{\epsilon_0} &= 1-\frac{\omega_{ep}^2-\omega_{eo}^2}{\omega^2-\omega_{eo}^2+i\gamma\omega},\end{aligned}$$

where ω_{*p} is the magnetic or electric plasma frequency and ω_{*o} is the magnetic or electric resonant frequency. As shown in [65], ϵ and μ are negative in the range 10.4 - 11 GHz. In this frequency band, the material exhibits a negative index of refraction. Many other investigators have since then confirmed negative refraction at microwave frequencies [22, 43].

In the work presented in this chapter, we specifically concentrate our attention to two assumptions employed when discussing LHM's: the first has to do with the requirement of a positive energy density, which in turn leads to the necessity of frequency dispersion in LHM's, and the second is related to the use of group velocity as the quantity which describes the behavior of a wave once inside a LHM. In response to these assumptions, we make two proposals: the first is that the positive energy density requirement should be relaxed, and the second is that the use of group velocity as the variable which determines physical information should be carefully reconsidered.

7.1 Maxwell's equations in left-handed materials

As previously mentioned, for existing naturally occurring materials, the positive sign of the square root in Eq. (7.2) is used. In [77], it is suggested that for a medium possessing simultaneous negative ϵ and μ, this convention must be reversed to satisfy energy considerations: the negative sign of the square root in Eq. (7.2) must be chosen instead. This statement seems to have no direct justification.

Snell's law is given by:

$$n_1 \sin\theta_1 = n_2 \sin\theta_2, \tag{7.3}$$

where n_1 is the index of refraction of the medium that the wave is incident from, and n_2 is that of the LHM. As per usual, θ_1 and θ_2 are respectively the angles of incidence and refraction at the interface. Equation (7.3) can be written in terms of the wave vectors as:

$$\mathbf{k}_1 \sin\theta_1 = \mathbf{k}_2 \sin\theta_2,$$

where we have used the relation:

$$n^2 = \frac{c^2}{\omega^2}\mathbf{k}\cdot\mathbf{k},$$

with ω being the frequency of the wave. The sign of the refractive index $n = n_1/n_2$, is determined by the relative sign between $\mathbf{k}_1$ and $\mathbf{k}_2$, which really depends not on the magnitude, but on the direction of the wave vectors in the two materials. In what follows, we show that the sign of this ratio turns out to be negative for materials described by simultaneously negative ϵ and μ.

We begin our calculation by considering a two-dimensional plane wave and letting the plane of incidence be the x-y plane. The interface between vacuum and the LHM is placed at $y = 0$. We are interested in the behavior of the wave vector $\mathbf{k}$ as the wave enters the LHM from vacuum. For this purpose, we let $\epsilon, \mu > 0$ for $y < 0$ and $\epsilon, \mu < 0$ for $y > 0$. There are two possible scenarios: the first is for the case in which the electric field is perpendicular to the plane of incidence and the second is for the case in which it is parallel to it. We study these two cases separately and show that the same results are obtained in either case.

7.1.1 Electric field perpendicular to plane of incidence

We consider here the electric field to be perpendicular to the plane of incidence (the x-y plane), and we assume that all fields have a time dependence given by $e^{-i\omega t}$. The wave vectors are assumed real but the fields are in general complex, with a magnitude and phase that change with position. The physical fields, of-course, are the real parts of these expressions. The plane wave can be described in terms of the electric field as:

$$\mathbf{E}(\mathbf{r},t) = \begin{cases} \mathbf{E}_{0I} e^{i(\mathbf{k}_I \cdot \mathbf{r} - \omega t)} + \mathbf{E}_{0R} e^{i(\mathbf{k}_R \cdot \mathbf{r} - \omega t)} & y < 0 \\ \mathbf{E}_{0T} e^{i(\mathbf{k}_T \cdot \mathbf{r} - \omega t)} & y > 0, \end{cases} \tag{7.4}$$

with:

$$\begin{aligned} \mathbf{k}_I &= k_x \hat{\mathbf{x}} + k_y \hat{\mathbf{y}} \\ \mathbf{k}_R &= k_x \hat{\mathbf{x}} - k_y \hat{\mathbf{y}} \\ \mathbf{k}_T &= k'_x \hat{\mathbf{x}} + k'_y \hat{\mathbf{y}}. \end{aligned}$$

$\mathbf{E}_{0I}$, $\mathbf{E}_{0R}$ and $\mathbf{E}_{0T}$ denote the complex amplitudes of the incident, reflection and transmission vectors. The wave vectors are related by

$$k_I v_1 = k_R v_1 = k_T v_2 = \omega,$$

with $v_1 = c$, and the fields are perpendicular to the propagation vector $\mathbf{k}$. Equation (7.4) can be rewritten as:

$$\mathbf{E}(\mathbf{r},t) = e^{-i\omega t} \begin{cases} e^{ik_x x} \left[E_{0I} e^{ik_y y} + E_{0R} e^{-ik_y y} \right] \hat{\mathbf{z}} & y < 0 \\ e^{ik'_x x} \left[E_{0T} e^{ik'_y y} \right] \hat{\mathbf{z}} & y > 0. \end{cases} \tag{7.5}$$

To calculate the magnetic field, we employ Faraday's Law, $\nabla \times \mathbf{E} = -\frac{\partial}{\partial t}\mathbf{B}$:

$$\left. \begin{aligned} -\frac{\partial}{\partial t} B_x = \frac{\partial}{\partial y} E_z = (ik_y) e^{-i\omega t} e^{ik_x x} \left[E_{0I} e^{ik_y y} - E_{0R} e^{-ik_y y} \right] \\ \frac{\partial}{\partial t} B_y = \frac{\partial}{\partial x} E_z = (ik_x) e^{-i\omega t} e^{ik_x x} \left[E_{0I} e^{ik_y y} + E_{0R} e^{-ik_y y} \right] \end{aligned} \right\} \quad y < 0$$

and

$$\left.\begin{aligned} -\frac{\partial}{\partial t}B_x = &\quad \frac{\partial}{\partial y}E_z = E_{0T}(ik'_y)e^{-i\omega t}e^{ik'_x x}e^{ik'_y y} \\ \frac{\partial}{\partial t}B_y = &\quad \frac{\partial}{\partial x}E_z = E_{0T}(ik'_x)e^{-i\omega t}e^{ik'_x x}e^{ik'_y y} \end{aligned}\right\} \qquad y > 0.$$

This translates to:

$$\left.\begin{aligned} B_x = &\quad \left(\frac{1}{\omega}\right)(k_y)e^{-i\omega t}e^{ik_x x}\left[E_{0I}e^{ik_y y} - E_{0R}e^{-ik_y y}\right] \\ B_y = &\; -\left(\frac{1}{\omega}\right)(k_x)e^{-i\omega t}e^{ik_x x}\left[E_{0I}e^{ik_y y} + E_{0R}e^{-ik_y y}\right] \end{aligned}\right\} \qquad y < 0$$

and

$$\left.\begin{aligned} B_x = &\quad \left(\frac{E_{0T}}{\omega}\right)(k'_y)e^{-i\omega t}e^{ik'_x x}e^{ik'_y y} \\ B_y = &\; -\left(\frac{E_{0T}}{\omega}\right)(k'_x)e^{-i\omega t}e^{ik'_x x}e^{ik'_y y} \end{aligned}\right\} \qquad y > 0,$$

or:

$$\mathbf{B}(\mathbf{r},t) = \frac{1}{\omega}e^{-i\omega t}\begin{cases} e^{ik_x x}\left[\begin{array}{c} (E_{0I}e^{ik_y y} - E_{0R}e^{-ik_y y})(k_y)\hat{\mathbf{x}} \\ -(E_{0I}e^{ik_y y} + E_{0R}e^{-ik_y y})(k_x)\hat{\mathbf{y}} \end{array}\right] & y < 0 \\ E_{0T}e^{ik'_x x}e^{ik'_y y}[k'_y\hat{\mathbf{x}} - k'_x\hat{\mathbf{y}}] & y > 0. \end{cases} \tag{7.6}$$

We can use Ampere's Law, $\nabla \times \mathbf{H} = \frac{\partial}{\partial t}\mathbf{D}$, or $\nabla \times \mathbf{B} = \epsilon\mu\frac{\partial}{\partial t}\mathbf{E}$, to arrive at the wave equation of the wave. The components are:

$$\begin{aligned} \epsilon\mu\frac{\partial E_x}{\partial t} &= -\frac{\partial B_y}{\partial z} \\ \epsilon\mu\frac{\partial E_y}{\partial t} &= \frac{\partial B_x}{\partial z} \\ \epsilon\mu\frac{\partial E_z}{\partial t} &= \frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y}. \end{aligned}$$

The only relevant equation is the third one. Using Eqs. (7.5) and (7.6), we obtain:

$$\omega^2 = \begin{cases} \frac{k_x^2+k_y^2}{\epsilon\mu} & y < 0 \\ \frac{k_x'^2+k_y'^2}{\epsilon'\mu'} & y > 0. \end{cases} \tag{7.7}$$

Before we can present a more detailed analysis of the behavior of the wave as it gets refracted into the LHM, we calculate the Poynting vector **S** associated with the electromagnetic field. The flux of energy of the electromagnetic wave in the direction of the energy flow is given by the real part of the complex Poynting vector, or $\mathbf{S} = \frac{1}{\mu}\mathbf{E} \times \mathbf{B^*}$, where the star superscript on **B** denotes complex conjugate[1]. For the form of the wave presented above,

$$\mathbf{S} = \frac{1}{\mu}\left[-E_z B_y^* \hat{\mathbf{x}} + B_x^* E_z \hat{\mathbf{y}}\right].$$

From Eqs. (7.5) and (7.6), the x and y components of the Poynting vector are found to be:

$$\left.\begin{aligned} S_x = & -\frac{1}{\mu}E_z B_y^* = \frac{1}{\omega}\left(\frac{k_x}{\mu}\right)(E_{0I})^2\left[1 + Re^{2ik_y y} + Re^{-2ik_y y} + R^2\right] \\ S_y = & \;\;\frac{1}{\mu}E_z B_x^* = \frac{1}{\omega}\left(\frac{k_y}{\mu}\right)(E_{0I})^2\left[1 - Re^{2ik_y y} + Re^{-2ik_y y} - R^2\right] \end{aligned}\right\} \quad y < 0 \tag{7.8}$$

and

$$\left.\begin{aligned} S_x = & -\frac{1}{\mu'}E_z B_y^* = \frac{1}{\omega}\left(\frac{k_x'}{\mu'}\right)(E_{0T})^2 \\ S_y = & \;\;\frac{1}{\mu'}E_z B_x^* = \frac{1}{\omega}\left(\frac{k_y'}{\mu'}\right)(E_{0T})^2 \end{aligned}\right\} \quad y > 0, \tag{7.9}$$

where $R = E_{0R}/E_{0I}$ and $T = E_{0T}/E_{0I}$.

At this point, it is important to notice that we have neither said anything about the signs of ϵ or μ, nor have we made any assumptions about the direction

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[1] For a detailed discussion of Poynting's Theorem, see [24].

of the wave vector inside the LHM. The physically significant information is hidden in the boundary conditions at the interface of the LHM. These ask for continuity of the normal components of **D** and **B**, and similarly for the parallel components of **E** and **H**. In other words, we ask for continuity in E_z, B_y and H_x. This gives:

$$\begin{aligned}(1+R)e^{ik_xx} &= Te^{ik'_xx} && (7.10)\\ k_x(1+R)e^{ik_xx} &= k'_xTe^{ik'_xx} && (7.11)\\ \left(\frac{k_y}{\mu}\right)(1-R)e^{ik_xx} &= \left(\frac{k'_y}{\mu'}\right)Te^{ik'_xx}, && (7.12)\end{aligned}$$

Equations (7.10) and (7.11) taken together lead to the condition:

$$k_x = k'_x, \tag{7.13}$$

and Eq. (7.11) becomes:

$$1 + R = T.$$

The reflection and refraction amplitudes are found to be:

$$\begin{aligned}R &= \frac{k_y/\mu - k'_y/\mu'}{k'_y/\mu' + k_y/\mu} && (7.14)\\ T &= \frac{2k_y/\mu}{k'_y/\mu' + k_y/\mu}. && (7.15)\end{aligned}$$

The last step to revealing the behavior of the wave vector as it enters the LHM, is to combine Eqs. (7.11), (7.12), and (7.13) to obtain:

$$\frac{1-R^2}{T^2} = \frac{\left(\frac{k'_y}{\mu'}\right)}{\left(\frac{k_y}{\mu}\right)}. \tag{7.16}$$

Here, $\mu = \mu_0 > 0$ is the permeability of vacuum and $\mu' < 0$ is that of the LHM. We notice that the left-hand side of Eq. (7.16) is positive if $|R| < 1$. Since k_y and μ

in Eq. (7.14) are both positive, the $|R| < 1$ condition is satisfied if $\frac{k_y}{\mu}$ and $\frac{k'_y}{\mu'}$ have the same sign (under the assumption that all the k's and μ's are real). Hence, since $\mu' < 0$, it is required that $k'_y < 0$, or that k_y and k'_y have opposite signs if μ and μ' have opposite signs. Equations (7.13) and (7.16) thus completely determine the direction of the transmitted wave vector $\mathbf{k}_T$.

7.1.2 Electric field parallel to plane of incidence

For completion, we now turn to the case of P-polarization for which the electric field is parallel to the plane of incidence, and show that the results produce conclusions which are identical to those presented in Section 7.1.1. In this case, the electric field contains a component that is perpendicular to the interface. The setup of the problem remains the same, but we now have to make use of the conditions $\hat{\mathbf{E}}_{0I} \cdot \hat{\mathbf{k}}_I = \hat{\mathbf{E}}_{0R} \cdot \hat{\mathbf{k}}_R = \hat{\mathbf{E}}_{0T} \cdot \hat{\mathbf{k}}_T = 0$ in order to calculate the incident, reflection, and transmission vectors. They are given by:

$$\begin{aligned}
\mathbf{E}_{0I} &= E_{0I}(k_y\hat{\mathbf{x}} - k_x\hat{\mathbf{y}}) \\
\mathbf{E}_{0R} &= -E_{0R}(k_y\hat{\mathbf{x}} + k_x\hat{\mathbf{y}}) \\
\mathbf{E}_{0T} &= E_{0T}(k'_y\hat{\mathbf{x}} - k'_x\hat{\mathbf{y}}).
\end{aligned}$$

In terms of the electric field, the wave can be written as:

$$\mathbf{E}(\mathbf{r},t) = \begin{cases} E_{0I}(k_y\hat{\mathbf{x}} - k_x\hat{\mathbf{y}})e^{i(k_x x + k_y y - \omega t)} - E_{0R}(k_y\hat{\mathbf{x}} + k_x\hat{\mathbf{y}})e^{i(k_x x - k_y y - \omega t)} & y < 0 \\ E_{0T}(k'_y\hat{\mathbf{x}} - k'_x\hat{\mathbf{y}})e^{i(k'_x x + k'_y y - \omega t)} & y > 0, \end{cases}$$

or:

$$\mathbf{E}(\mathbf{r},t) = e^{-i\omega t}\begin{cases} e^{ik_x x}\begin{bmatrix} [E_{0I}e^{ik_y y} - E_{0R}e^{-ik_y y}](k_y)\hat{\mathbf{x}} \\ -[E_{0I}e^{ik_y y} + E_{0R}e^{-ik_y y}](k_x)\hat{\mathbf{y}} \end{bmatrix} & y < 0 \\ e^{ik'_x x}E_{0T}(k'_y\hat{\mathbf{x}} - k'_x\hat{\mathbf{y}})e^{ik'_y y} & y > 0. \end{cases}$$

The magnetic field is found to be:

$$\mathbf{B}(\mathbf{r},t) = \frac{e^{-i\omega t}}{-\omega}\begin{cases} e^{ik_x x}\big(k_x^2 + k_y^2\big)(E_{0I}e^{ik_y y} + E_{0R}e^{-ik_y y})\hat{\mathbf{z}} & y < 0 \\ e^{ik'_x x}E_{0T}\big(k_x'^2 + k_y'^2\big)e^{ik'_y y}\hat{\mathbf{z}} & y > 0. \end{cases}$$

The wave equation can be calculated for this case and, as expected, it is found to be identical to Eq. (7.7). The components of the Poynting vector are given by:

$$\left.\begin{aligned} S_x = {} & \frac{1}{\mu}E_y B_z^* = \frac{1}{\omega}\left(\frac{k_x}{\mu}\right)\big(k_x^2 + k_y^2\big)(E_{0I})^2\big[1 + Re^{2ik_y y} + Re^{-2ik_y y} + R^2\big] \\ S_y = {} & -\frac{1}{\mu}E_x B_z^* = \frac{1}{\omega}\left(\frac{k_y}{\mu}\right)\big(k_x^2 + k_y^2\big)(E_{0I})^2\big[1 + Re^{2ik_y y} - Re^{-2ik_y y} - R^2\big] \end{aligned}\right\} \quad y < 0 \tag{7.17}$$

and

$$\left.\begin{aligned} S_x = {} & \frac{1}{\mu'}E_y B_z^* = \frac{1}{\omega}\left(\frac{k'_x}{\mu'}\right)\big(k_x'^2 + k_y'^2\big)(E_{0T})^2 \\ S_y = {} & -\frac{1}{\mu'}E_x B_z^* = \frac{1}{\omega}\left(\frac{k'_y}{\mu'}\right)\big(k_x'^2 + k_y'^2\big)(E_{0T})^2 \end{aligned}\right\} \quad y > 0. \tag{7.18}$$

The boundary conditions ask for continuity in E_x, D_y, and H_z. These give:

$$k_y(1 - R)e^{ik_x x} = k'_y T e^{ik'_x x} \tag{7.19}$$

$$\epsilon k_x(1 + R)e^{ik_x x} = \epsilon' T(k'_x)e^{ik'_x x} \tag{7.20}$$

$$\frac{1}{\mu}\big(k_x^2 + k_y^2\big)(1 + R)e^{ik_x x} = \frac{1}{\mu'}\big(k_x'^2 + k_y'^2\big)T e^{ik'_x x}, \tag{7.21}$$

Equations (7.7), (7.20), and (7.21) taken together lead us back to Eq. (7.13), or:

$$k_x = k'_x, \tag{7.22}$$

and this completely determines the sign of k'_x to be the same as that of k_x, just like in the Section 7.1.1. The sign of k'_y can be determined by combining together Eqs. (7.19), (7.20), and (7.22). This gives us:

$$\frac{\epsilon' k'_y}{\epsilon k_y} = \frac{1 - R^2}{T^2}, \tag{7.23}$$

which is the same as Eq. (7.16) except that every μ is replaced by a corresponding $1/\epsilon$. Again, to make $|R| < 1$ in Eq. (7.23) when ϵ and ϵ' have opposite signs, one needs k_y and k'_y to have opposite signs. Hence, once again, $k'_y < 0$.

The reflection and transmission amplitudes are found to be:

$$\begin{aligned} R &= \frac{\epsilon' k'_x k_y - \epsilon k_x k'_y}{\epsilon k_x k'_y + \epsilon' k'_x k_y} \\ T &= \frac{2\epsilon k_x k_y}{\epsilon k_x k'_y + \epsilon' k'_x k_y}. \end{aligned}$$

A great deal of physically important information is contained in the ratios $\frac{k'_x}{\mu'}$, and $\frac{k_y}{\mu'}$ appearing in Eqs. (7.9) and (7.18). Since μ is positive, Eqs. (7.8) and (7.17) state that the Poynting vector is parallel to the wave vector in the region $y < 0$. However, as the sign of the permeability changes from positive to negative as the wave moves from vacuum to the LHM, the Poynting vector becomes antiparallel to the wave vector in the region $y > 0$, as shown by Eqs. (7.9) and (7.18). This result was obtained in [77] by using different arguments. The situation is depicted in Fig. 7.1. Notice that, as expected, the energy flux is away from the interface for $y > 0$.

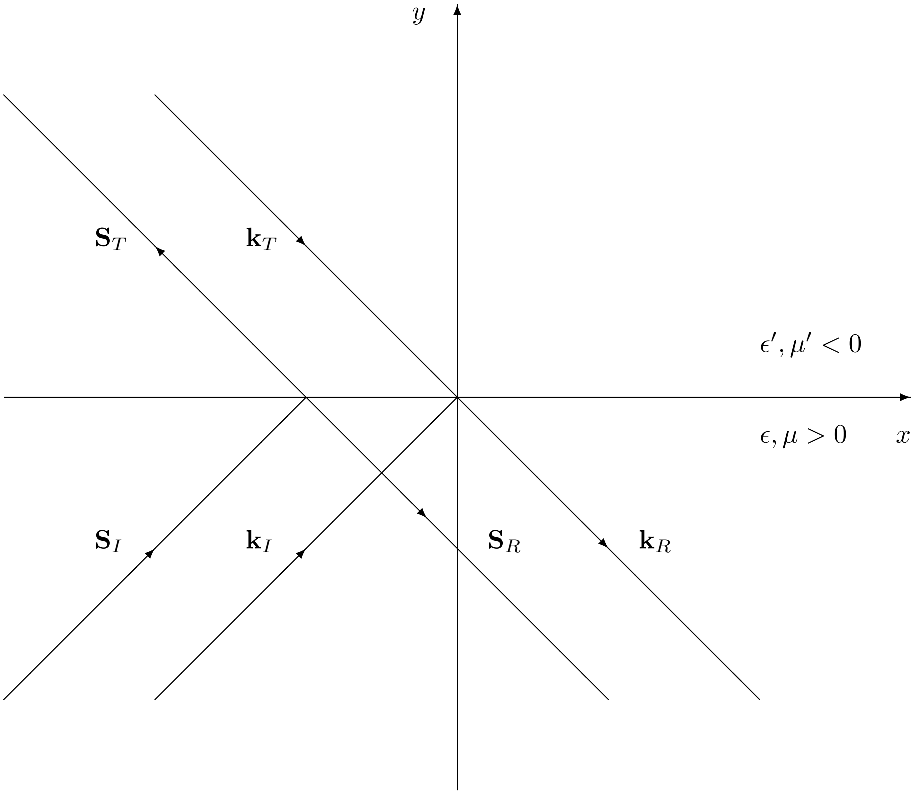

Figure 7.1: Ray diagram for the behavior of a plane wave as it propagates into a left-handed medium placed at $y = 0$. The “ray” is shown in terms of the Poynting vector as well as the wave vector.

7.2 Negative energy density and frequency dependence

In all literature available up to date, it has been assumed that negative refractive materials are necessarily frequency dependent. In this section, we propose an alternative to this assumption.

Consider the energy density of the electromagnetic wave in a non-dispersive medium (Eq. (22) in [77]):

$$W = \epsilon E^2 + \mu H^2. \tag{7.24}$$

In [77] it is argued that the sign of Eq. (7.24) should be positive at all times. It is further suggested that, since simultaneously negative values of ϵ and μ would make $W < 0$, Eq. (7.24) should be replaced with the expression for the energy density in a dispersive medium (Eq. (23) in [77]):

$$W = \frac{\partial(\epsilon\omega)}{\partial\omega} E^2 + \frac{\partial(\mu\omega)}{\partial\omega} H^2. \tag{7.25}$$

In order to have $W > 0$ in Eq. (7.25), it is required that $\frac{\partial(\epsilon\omega)}{\partial\omega} > 0$, and $\frac{\partial(\mu\omega)}{\partial\omega} > 0$. More importantly, because of the positive energy density requirement, negative refraction can be realized only when there is frequency dispersion. As a final remark, it is claimed that the partials in Eq. (7.25) do not in general mean that ϵ and μ cannot be simultaneously negative, but for them to hold, it is necessary that ϵ and μ are frequency dependent.

There are many situations in physics where energy assumes negative values. Two of the most well-known examples are those arising from the Klein-Gordon and the Dirac relativistic wave equations. Both these equations admit negative energy solutions which are not realized in nature. This gives an apparently fatal difficulty, since an external perturbation can cause a particle with energy greater than its rest mass energy mc^2 to make a radiative transition to a state of negative energy less than mc^2. In 1930, Dirac proposed a way out of this difficulty by suggesting that, for electrons, there are states in nature that admit negative energy, but they are all full. Since, according to the Pauli exclusion principle, only one electron is allowed in each state, transitions from positive to negative energy states are only allowed if there is a mechanism that empties the already full negative states. In this picture, the vacuum state consists of an infinite sea of electrons filling all the negative energy states and all the positive energy states are empty. It is possible for an electron in the negative sea to acquire energy greater than $2mc^2$ and make a transition to a positive energy state with some value greater than mc^2. This transition leaves behind a *hole* in the sea of negative-energy states. Measured with respect to the vacuum, this hole appears to have a positive charge $(+e)$ and positive energy; it can therefore be interpreted as a *positron.* This is how Dirac predicted the existence of positrons, which were indeed discovered in 1933 by C.D.Anderson.

The Dirac field with the negative energy sea all filled, has difficulties with relativistic invariance. The problem presents itself when the negative energy states are reinterpreted as holes. For an extensive discussion, see [15]. However, there are other situations in which negative energy presents itself. Let's consider the case in which there is a region in space in which the energy density W associated with the motion of particles is negative. Such a question was considered in [2] for the case of tachyons, particles capable of overcoming the light barrier. Consider being in a frame S which is at rest. Also suppose that in that frame, a tachyon is observed to be emitted by a source and absorbed a while later by a sink. It was shown that, for an observer in some other frame S' moving with velocity w with respect to frame S, these particles may appear to have negative energy. In addition, to the observer in the S' system, the negative-energy particle will appear to have been absorbed first and emitted later. At the time, this phenomenon raised serious objections to the possible existence of tachyons. To resolve this difficulty, the authors proposed a *reinterpretation principle.* According to this principle, a negative-energy particle that has been absorbed first and emitted later, is nothing else but a positive-energy particle emitted first and absorbed later, a perfectly normal situation.

It also turns out that, for the case of tachyons, the velocity is antiparallel to the momentum. This is analogous to what we observe in negative refractive index materials: the Poynting vector is antiparallel to the wave vector. As a parallel to the case of tachyons, it looks like, inside the LHM, the wave hits the interface before it is emitted by its source. By an analogous reinterpretation technique, we can think of a negative-energy wave propagating in one direction as a positive-energy wave propagating in the opposite direction.

Allowing the existence of negative energy solutions has consequences which contradict the claims in [77]. Namely, allowing W to be negative means that the partials in Eq. (7.25) are no longer restricted to be positive. More importantly, however, Eq. (7.24) need not be replaced by Eq. (7.25), and the requirement that the medium be dispersive if negative refraction can occur is no longer necessary. One could in fact ask the question of what happens in certain regions of a material in which the absorption bands are far enough apart such that the region in-between them is essentially non-dispersive for a quasi-monochromatic pulse. Once negative energy solutions are accepted, it seems like there is no fundamental reason justifying the rejection of negative refraction in non-dispersive materials.

Dispersion and the role of group velocity

We finish this chapter with a review of the fundamentals of the phenomenon of dispersion and a discussion of the use of group velocity to describe the behavior of a wave inside a LHM. In Section II of [77], the author states that in negative index materials, $\mathbf{S}$ and $\mathbf{k}$ are antiparallel, and suggests that such materials must have negative group velocity. The assumption here is that the so-called group velocity $\mathbf{v}_g$ is in the same direction as the Poynting vector, which is in turn antiparallel to $\mathbf{k}$ and also to the phase velocity $\mathbf{v}_p$. It is also suggested that $\mathbf{v}_p$ is opposite to the energy flux, which is taken to be $\mathbf{S}$ or $\mathbf{v}_g$ interchangeably. In the discussion that follows, we claim that the use of group velocity as presented in [77] may not be inevitable, but we wish to point out that a careful reinterpretation of a negative energy mode is as we have suggested. The notion of group velocity should perhaps be used very carefully, if at all.

The variation of the refractive index with wavelength (or frequency) constitutes the phenomenon of dispersion. For a detailed derivation of the characteristic frequency dispersion equations, we refer the interested reader to [4] and [24], in which discussions of a simplified model of a dispersive medium can be found. In the case of *normal* dispersion n increases with ω, while in the case of *anomalous* dispersion n decreases with ω and has a significant imaginary part.

It is found that if one were to plot a graph of n versus λ for a range of different optical materials, that curve would differ in detail from one material to the next, but all curves would have the same general shape. Curves representative of normal dispersion are characterized by the following facts: n increases with decreasing λ, the rate of increase $dn/d\lambda$ rises at shorter wavelengths, the larger the index of refraction of a certain substance, the steeper $dn/d\lambda$ is for a given wavelength, and the curve of one substance cannot in general be obtained from that of another substance by a simple change in the scale of the ordinates. The magnitude of n is in general quite different for various substances, but its change with wavelength shows the characteristics described above.

Anomalous dispersion is seen when the index of refraction is measured for substances like quartz in the infrared region of the spectrum. In that case, the dispersion curve begins to deviate significantly from that which describes normal dispersion. More specifically, the measured value of n decreases more and more rapidly with increasing λ, until it reaches a region in the infrared where light ceases to be transmitted at all. This region of selective absorption is known as the absorption band, and its position is characteristic of the material in question. Since the substance does not transmit radiation of the wavelength in the absorption band, n cannot usually be measured in this region. The index of refraction is found to be higher for the long wavelength side of the absorption band, and as one moves further away from the band, n decreases rapidly at first and more slowly later.

Anomalous dispersion was first observed with materials whose absorption bands fall in the visible region of the spectrum. However, it was soon discovered that transparent substances like glass and quartz possess regions of selective absorption in the infrared and ultraviolet regions, and therefore show anomalous dispersion in those areas. It turns out that no substance exists which does not exhibit anomalous dispersion at some wavelengths, making the term “anomalous” inappropriate. This phenomenon, far from being anomalous, is perfectly general. The so-called “normal” dispersion is seen only in the frequency region between two absorption bands, and fairly far removed from them. Nonetheless, the term “anomalous dispersion” has been retained for historical reasons.

It is not uncommon for some positive index materials to exhibit regions in which $\mathbf{v}_p > 0$ and $\mathbf{v}_g < 0$ [16, 42]. In this sense, there is nothing special about negative index materials, contrary to the assertion that LHM's are materials with negative group velocity. To make things more transparent, let us recall that the phase and group velocity of a wave are related by:

$$v_g = v_p + k\frac{dv_p}{dk} = v_p - \lambda\frac{dv_p}{d\lambda}, \tag{7.26}$$

where the relation $k = 2\pi/\lambda$ has been used to arrive at the second part of the equation above. Equation (7.26) can also be expressed in terms of the refractive index n as:

$$v_g = \frac{\partial \omega}{\partial k} = \frac{c}{\mathrm{Re}(n) + \omega \frac{\partial \mathrm{Re}(n)}{\partial \omega}}. \tag{7.27}$$

In the fictitious case of a complete absence of dispersion, the group velocity is identical to the phase velocity in both magnitude and direction. However, the sign of the group velocity can be positive or negative depending on the sign of the second term in the denominator of Eq. (7.27) and its magnitude with respect to Re(n). It should thus be expected that the relative sign between $\mathbf{v}_p$ and $\mathbf{v}_g$ varies in different frequency regions of the same material, irrespective of the sign of its refractive index. In fact, all four sign combinations between $\mathbf{v}_p$ and $\mathbf{v}_g$ have been verified experimentally for a negative index material [12]. It is important to note at this point that nowhere in the above discussion has the Poynting vector been mentioned.

Even though it is unlikely that a material in which dispersion is absent entirely exists naturally, there surely must be frequency regions within materials for which dispersion is so small that it can be thought of as negligible. According to [77], negative refraction is not allowed in those regions. Based on fundamental physical reasoning, we suggest an alternative to this proposal.

Since no assumptions of the nature of the medium were made in deriving Eq. (7.7), we are in a position to study the behavior of the wave vector as a function of frequency in the region of interest for any medium of our choice. Below, we present two cases: in the first, we consider the unlikely case of a non-dispersive medium in which ϵ and μ are frequency independent, and in the second, we consider the case of a medium with a simple frequency dependence of the form $\epsilon(\omega) = \epsilon_0 \left(1 - \frac{\omega_p^2}{\omega^2}\right)$ and $\mu(\omega) = \mu_0 \left(1 - \frac{\omega_p^2}{\omega^2}\right)$, where ω_p is the constant plasma frequency. We focus our attention to the region $y > 0$ for the case where the electric field in perpendicular to the plane of interface, such that $k_x = k_x'$.

As mentioned previously, even though the existence of a medium in which dispersion is absent entirely is unlike, there are, realistically, frequency regions within materials for which dispersion can be thought of as negligible. We present here the case of a non-dispersive medium as an illustrative example corresponding to those regions inside the medium in which dispersion is so small that it can be neglected. In that case, Eq. (7.7) becomes:

$$k_y'^2 c^2 = \omega^2 \left[\frac{\epsilon' \mu'}{\epsilon_0 \mu_0} - \sin^2 \theta_i \right] , \tag{7.28}$$

with ϵ', μ' negative constants and $\epsilon' \mu' / \epsilon_0 \mu_0 > 1$. Here, θ_i is the incident angle of the wave, and k_x' has been replaced with $\frac{\omega}{c} \sin \theta_i$. Equation (7.28) has two possible solutions:

$$k_y' c = \pm \omega \sqrt{\frac{\epsilon' \mu'}{\epsilon_0 \mu_0} - \sin^2 \theta_i}.$$

The behavior of the y-component of the wave vector as a function of frequency is a simple linear relation and is shown in Fig. 7.2 for an incident angle of $\theta_i = 30^\circ$ and positive ω.

Following the results of the calculations of Section 7.1, the physical region of interest is that in which $k_y' < 0$. As an aside, note that for this region, $\mathbf{v}_p$ and $\mathbf{v}_g$ are negative and parallel. This is of no surprise, of-course, since in the absence of dispersion, the group velocity of the wave is precisely its phase velocity. At the same time, the energy flux is positive.

We proceed to study the same problem in the case where ϵ and μ are described by a simple frequency dependence of the form $\epsilon(\omega) = \epsilon_0 \left(1 - \frac{\omega_p^2}{\omega^2}\right)$ and $\mu(\omega) = \mu_0 \left(1 - \frac{\omega_p^2}{\omega^2}\right)$, where ω_p is the constant plasma frequency. This model has been treated earlier in [23], where a detailed discussion of arguments based on group velocity can be found. Under this assumption, equation (7.7) takes the form:

$$k_y'^2 c^2 = \omega^2 \left[\left(1 - \frac{\omega_p^2}{\omega^2}\right)^2 - \sin^2 \theta_i \right] . \tag{7.29}$$

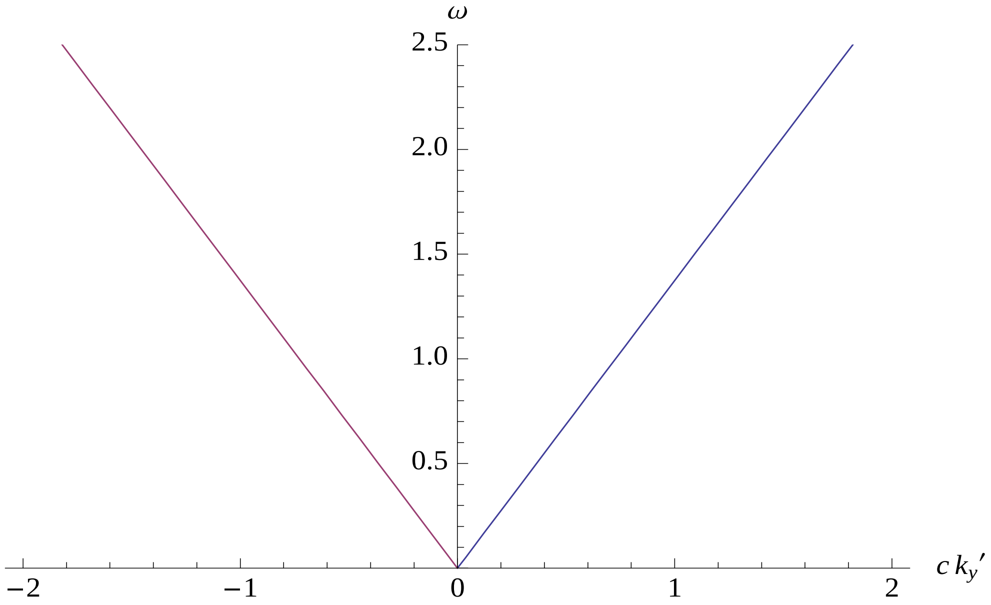

Figure 7.2: Behavior of the y-component of the refracted part of the wave vector as a function of frequency for $y > 0$ and ϵ, μ negative constants and $\epsilon\mu/\epsilon_0\mu_0 > 1$. The wave is incident at an angle of 30°.

Once again, there are two possible solutions to Eq. (7.29):

$$k_y' c = \pm\omega\sqrt{\left(1 - \frac{\omega_p^2}{\omega^2}\right)^2 - \sin^2\theta_i}. \tag{7.30}$$

A plot of the real values of the y-component of the wave vector as a function of frequency for the case where ϵ and μ have this particular frequency dependence is shown in Fig. 7.3.

Figure 7.3 displays all four solutions of Eq. (7.30). The upper branch has $\frac{\omega}{\omega_p} > 1$ and corresponds to ϵ and μ positive. Similarly, the lower branch has $\frac{\omega}{\omega_p} < 1$ and corresponds to ϵ and μ negative. Again, we are interested in the region in which $k_y' < 0$. Figure 7.3 shows that for positive index materials $\mathbf{v}_p$ and $\mathbf{v}_g$ are positive and parallel, while for negative index materials, $\mathbf{v}_p < 0$ and $\mathbf{v}_g > 0$. Again, the

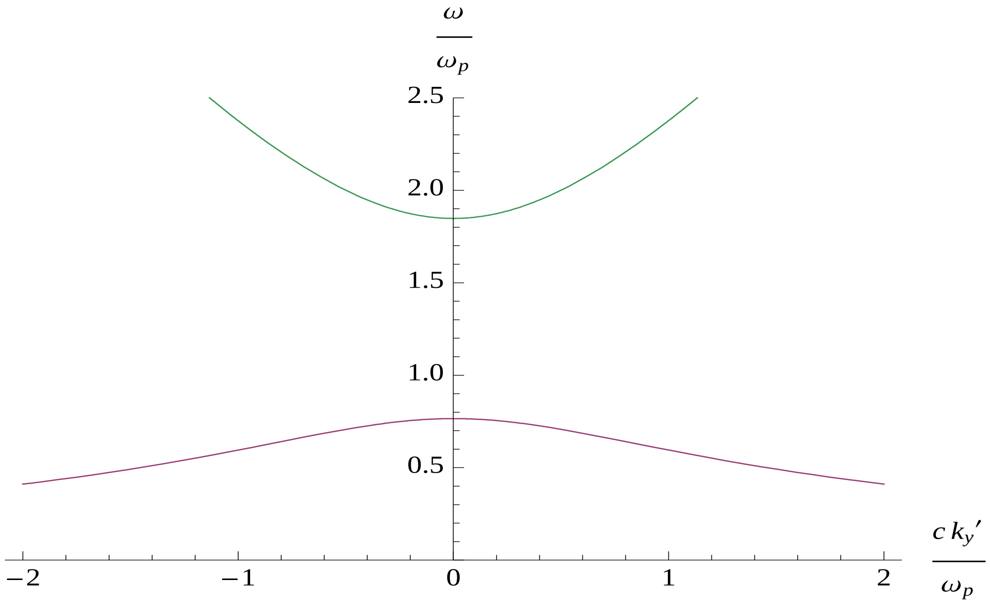

Figure 7.3: Behavior of the y-component of the refracted part of the wave vector as a function of frequency for $y > 0$ and $\frac{\epsilon}{\epsilon_0} = \frac{\mu}{\mu_0} = 1 - \frac{\omega_p^2}{\omega^2}$. The wave is incident at an angle of 45°.

energy flux is positive in both cases.

Chapter 8

Concluding remarks and future directions

8.1 Relaxation in harmonic oscillator systems

In the first part of this dissertation, we explicitly calculated the time evolution of an initially uncoupled harmonic oscillator system, under the repeated application of an interaction Hamiltonian for successive time intervals τ. The bipartite system under consideration was composed of a physical system of interest, and the environment with which this system was in contact. The results were obtained exactly by using iterative methods and without employing perturbation theory. We showed that after enough periodically repeated applications of the interaction Hamiltonian, the physical system of interest came to equilibrium with its environment - *if* the frequencies of the two subsystems were equal - at an effective temperature which was equal to the initial temperature of the environment. We also showed that when the frequencies of the two subsystems were unequal, the physical system of interest approached but never attained the environment's temperature.

It was shown that the steady state of our system was obtained through a series of transient Maxwell-Boltzmann distributions, and the new steady state satisfied the condition $\omega_1\theta_1(\infty) = \omega_2\theta_2(0)$. It was concluded that the selection rules imposed by the interaction Hamiltonian overrode statistical mechanical effects. The results were first obtained for the case where the physical system of interest represented by a single harmonic oscillator was coupled to an environment composed of a single harmonic oscillator. These results were extended to the case where the same single harmonic oscillator system was coupled to an environment composed of at least two harmonic oscillators. To obtain the most general open evolution of the system of interest, the situation was generalized to the case where the environment was composed of N harmonic oscillators.

An important ingredient introduced in our model was the "refresh" procedure. After applying a constant interaction Hamiltonian to our initially uncoupled bipartite system, a "refreshing" mechanism was performed. This mechanism corresponded to the assumption that there were no fixed phase relationships between the physical system of interest and the environment surrounding it, while at the same time, the phase relationships between the number states of each individual oscillator were definite. In addition, it was assumed that we had no knowledge about the occupation numbers of each of the modes in the second system and so averaging over all these occupation numbers was performed.

The fact that the total number of particles was conserved by definition of the total Hamiltonian of our model, and the fact that the initial density matrix was diagonal in the number basis $\{|n_1, n_2, \cdots, n_N\rangle\}$ of the harmonic oscillators, forced the evolved reduced density matrix $\rho^S(n\tau)$ with $n = 0, 1, 2, \cdots, \infty$ to be diagonal in its respective number basis $\{|n_1\rangle\}$. In turn, this allowed for the composite system density matrix after the "refreshing" to be written as a product state of the new system and environment states.

The results and consequences obtained in this dissertation were dependent on the assumptions put forth in the “interact-refresh-repeat” relaxation-generating model, along with the chosen interaction Hamiltonian. When analyzing multi-stage processes, it is often a good assumption to use the Markov approximation. This approximation ignores the built-up of correlations between the system and its environment and is valid for short times. The irreversible evolution of a system in contact with an environment is obtained, provided that the decay time or the time it takes for correlations with the environment to become important are much shorter than the typical relaxation times of the two subsystems. These assumptions taken together lead to exponential decays. Nonetheless, there are many situations in physics in which the use of the Markov approximation may be inappropriate. An example is seen in the quantum Zeno effect [33], in which the decay of a system at very short times is not exponential in nature.

Our results were also unique in the sense that the initial composite system-environment state was assumed to be in a tensor product of the two subsystems. In other words, initial correlations were ignored. In many cases of practical interest, this is a reasonable assumption. When an experimentalist prepares a system in a specified state and has complete control over the initial state of interest, all correlations between the system and the environment are undone. Ideally, the destruction of all correlations will leave the system in a pure state. In practice, however, uncoupling a system from its environment is in general very difficult and it is very rarely accomplished experimentally. Quantum systems interact constantly with their environments, leading to the built-up of correlations. One way in which these correlations express themselves is via the exchange of heat between the system and its environment.

One can then ask the following questions:

- *How will our results change if:*
    - *initial system-environment correlations are assumed?*

  - *the interaction Hamiltonian can allow for free evolution of the individual parts (i.e. it can allow for the interaction coupling to have an explicit time-dependence?)*

- *What are the conditions (if any) under which the above models can be treated as Markov processes? And if none, how can non-Markovian effects be incorporated in the problem?*

The above are just a few of the questions which remain unanswered. Nonetheless, we hope that the work which was presented in this dissertation can contribute to the foundations of the study of Markovian processes in the context of open quantum systems.

8.2 Wave propagation in left-handed materials

In the second part of this dissertation, we examined the response of a plane, monochromatic electromagnetic wave incident on a left-handed material from vacuum, by explicitly solving Maxwell's equations. The physically significant information was explored by matching the boundary conditions at the interface. We proposed that negative energy solutions should not be rejected on the grounds of being unphysical, and examined the implications arising from such a change. We specifically focused our attention on the claim that if negative energy solutions are accepted, negative refraction can be allowed to occur in frequency regions within a material for which dispersion is essentially negligible. We further examined the role of group velocity and suggested that all possible sign combinations between the phase and the group velocity of a wave should be expected in all materials, regardless of the sign of the refractive index. To finish, we solved the wave equation for a wave incident on a left-handed medium from vacuum for two extreme cases: in the first, we assumed the absence of dispersion, and in the second, we assumed the high-frequency limit.

The original prescription for a sub-wavelength array of thin metallic wires combined with resonant metallic rings has been extensively investigated, and negative refraction at microwave frequencies has been confirmed by several investigators. In addition, a great deal of effort has been put in trying to create a material with a negative refractive index for visible light. In fact, in 2000, Notomi showed that negative refraction should be expected to occur in photonic crystals for a certain range of frequencies [40]. Photonic crystals are periodic structures built on the scale of the optical wavelength, which allow only certain wavelengths to pass through. Essentially, they are structures in which the refractive index can be controlled by their band structure. The nice thing about photonic crystals, other than the fact that they are built within the visible region, is that they have significantly reduced losses. Many researchers have already explored negative refraction and Cherenkov radiation using photonic crystals [10, 11, 14, 30, 31, 41, 44, 45]. All possible sign combinations between phase and group velocities were observed in these materials [34].

One problem with the original structures presented is that they were not suitable for practical microwave applications because of their excessive loss and narrow bandwidth. Caloz *et al.* introduced a transmission line approach of left-handed materials and proposed an artificial left-handed transmission line with microstrip components including interdigital capacitors and shorted stub inductors [7]. Since then, researchers have arrived at the circuit equivalent of a negative index material using transmission lines [13, 19, 29, 66]. It is very important to note here that experiments involving transmission-line devices demonstrate only moderate dispersion with no noticeable increase in absorption. It is understood that it would be a challenging (if not impossible) task to experimentally study materials in which dispersion is negligible. However, the recent approaches to negative refraction involving photonic crystals and circuit models indicate a promising future as far as the arguments on the necessity of dispersion put forth in this dissertation.

Inevitably, the implications accounting to the wave propagation inside a left-handed medium have challenged our current understanding of optics. To a physicist, the peculiar behavior of a wave inside a left-handed material constitutes counter-intuitive phenomena. Theoretical questions about the possibility of the fabrication of perfect lenses and invisibility cloaks, as well as the apparent violation of causality are just a few of the subjects which have raised interesting theoretical debates between researchers in this field [21, 49, 71, 73, 84]. Even though theoretical questions of this nature still remain unanswered, we hope that the suggested inclusion of negative energy solutions within the context of wave propagation inside left-handed media can contribute to the understanding of some of the aspects of the peculiar phenomena observed in these novel structures.

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Vita

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