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Evolution of a 1D Bipartite Fermionic Chain Under Influence of a Phenomenological Dephasing

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Dedicated to my eternal master, Erlon Santana.

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Resumo

Em sistemas microscópicos, grandezas como calor e trabalho devem ser tratadas como variáveis aleatórias. Neste trabalho foram estudados os fluxos de calor e de partículas entre dois sistemas unidimensionais fermiônicos A e B, inicialmente preparados separadamente em equilíbrio térmico com reservatórios de calor e partículas preparados a dfiferentes temperaturas e diferentes potenciais químicos. Calculando a evolução da matriz densidade, foram analisadas as implicações da presença de um ruído de *dephasing* no sistema, tais como a termalização, a produção de entropia e a evolução da informação mútua como uma forma de analisar a correlação entre os sistemas. Além disso, foi estudado também uma forma do teorema de flutuação do calor no caso onde há fluxo de partículas.

Palavras chave: Sistemas Quânticos Abertos, Teorema de Flutuação, Equação Mestra de Lindblad,Informação Mútua, Produção de Entropia, Fluxo de Calor, Fluxo de Partículas

Abstract

In microscopic systems, heat and work must be treated as random variables. In this work I studied the fluxes of heat and particles between two unidimentional fermionic systems A and B, initially prepared in thermal equilibrium with a reservoir of particles and heat, kept at different temperatures and chemical potentials. Computing the evolution of the density matrix, the implications of the presence of a *dephasing* noise in the system were analyzed, such as thermalization, entropy production and the evolution of mutual information as a way to analyze the correlation between the systems. Moreover, a shape for fluctuation theorems of the heat in the case where there is also a flux of particles and its validity was also studied.

Keywords: Open Quantum Systems, Fluctuation Theorem, Lindblad Master Equation, Mutual Information,Entropy Production, Heat Flux, Particle Flux

Contents

Chapter 1

Introduction

The thermodynamics of macroscopic processes, in general, makes part of our intuition since thermodynamical phenomena occur everywhere in our daily lives. For example, if we put a cup of hot tea over a table and let it sit, we know that it will be cooled until it reaches room temperature. After a sufficiently long time has elapsed, we say the hot tea has reached *thermal equilibrium* with its environment. Moreover, our everyday experience also tells us that this process is irreversible, once we do not expect that the reverse occurs [1].

The equilibrium properties of thermodynamic systems are fully characterized by a handful of variables, such as energy, volume and number of particles. Moreover, equilibrium allows us to readily separate changes in the energy ΔU as stemming from the work W performed in a system and the heat Q exchanged with a reservoir, as [2]

$$\Delta U = Q + W \tag{1.1}$$

which is the first law of thermodynamics.

Many phenomena in classical thermodynamics can be adequately treated using only equilibrium concepts. What this means is that the processes are driven so slowly in such way that the system reaches the new equilibrium almost instantly. Although it seems a bit strange, because most of the processes do not occur at this speed, thermodynamics of equilibrium gives us important results, such as the limit of efficiency of a thermal engine, given by Carnot [3].

Despite these important results, equilibrium thermodynamics is not capable of explaining other important quantities, such as the flux of particles and heat. For example, in biology, it is much more interesting to study nonequilibrium processes such as sodium and potassium pump, which change the concentration of sodium and potassium in a intracellular medium, than to study the eventual equilibrium that every leaving creature eventually reach. So in the context of thermodynamics we can imagine that such fluxes can tell us about the thermalization and *how* it thermalizes.

In the standard thermodynamic formulation, the thermodynamic quantities are assumed to be deterministic quantities, not prone to fluctuations. That, of course, is a consequence of the large number of particles in macroscopic systems, which make the fluctuations negligibly small compared to the average [4]. Thus, in our daily lives, we do not observe important fluctuations, but for a small number of particles these fluctuations become important. Thereby, once these fluctuations become important, quantities such as heat and work must be treated as random variables. A clear example of this was shown in reference [5], where the authors studied the work necessary to fold and unfold a RNA molecule. As a result, they find that due to thermal fluctuations, the work required changes each time the experiment is repeated. It thus makes sense to speak about the probability of work.

Fluctuation theorem refers to a collection of theoretical preditions, which can be roughly summarized by:

$$\frac{p(+\Sigma)}{p(-\Sigma)} = e^{\Sigma}, \tag{1.2}$$

where $p(\Sigma)$ is the probability that a certain amount of entropy Σ was produced during the process of duration τ [6]. Historically, the first proved fluctuation theorem is of autorship of Crooks [7]. In his paper he showed that, for a system prepared at a thermal state, the rate between the probability of performing a work W and the probability of the inverse process occurs with a work $-W$ is given by [7]

$$\frac{p_F(+W)}{p_B(-W)} = e^{\beta W}. \tag{1.3}$$

With this on hands, he was also able to obtain the Jarzynski's equality [8]

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}, \tag{1.4}$$

in which ΔF is the variation of free energy in the system. Such equality was a groundbreaking result, since most thermodynamical relations are inequality and it is valid for arbitrary out of equilibrium systems.

The example used here a short time ago was an article of 2005 that reported an experimental verification of Crooks's fluctuation theorem for objects as bigs as RNA ribbons [5], as used as example before. In 2004, Jarzynski provided us a classical and a quantum version of fluctuation theorems for heat based on the time-reversal property [6].His fluctuation theorem has been extensively applied for different systems [9, 10, 11] and experimentally verified [12, 13].

It has been shown recently that it is possible to construct thermodynamics for systems of few particles using quantum mechanics as a tool [14]. This conection between the quantum mechanics and thermodynamics is called *quantum thermodynamics* [15]. Thanks to quantum thermodynamics, it has been possible to describe microscopic systems such as spins and chains of harmonic oscillators. [16, 17, 18] .

Usually, an energy variation of a given system is divided between heat and work. Heat is described as a chance of the probability distribution of the states of the quantum systems, while work is described as a change in the eigenvalues of the system. This approach allowed us to consider purely quantum characteristics, as a superposition of states, in the treatment of such quantities [19]. Moreover, quantum versions for fluctuations theorems were done and verified experimentally [5, 20].

Correlation functions are effective ways of representing the dynamics of a system. In the context of quantum mechanics , they are generally used to analyze time-dependent processes with stochastic or irreversible dynamics [21]. Moreover, these correlations play a significant role in efficient quantum comunication and and quantum computational tasks, while in quantum many-body systems, they help us to undestand cooperative phenomena [22].

Quantum thermodynamics is also the responsible to study how the entropy production emerges. A problem then emerges from the fact that for unitary evolutions there is no entropy production. Looking at a simple example of an interaction of two closed gases of different temperature, but both with contact with a diatermic wall between them, we know from the classical thermodynamics that the systems will change heat, reach the equilibrium and entropy will be produced.

Superposition of states is one of the pillars of quantum mechanics. Such superpositions are a kind of signature of the quantumness of the system and may be directly ou indirectly determined experimentally, as done in the Stern-Gerlach or in double-slit experiments [23]. In our daily lives, where the classical physics dominates the explanations of the processes, we do not observe such superpositions. Such fact may be explained with the help of decoherence mechanisms.

In the context of *open quantum systems*, one responsible for the loss of coherence is *dephasing*. Dephasing is a mechanism that makes the coherence of the system, and consequently the superposition states in a certain basis, decay leading to a complete mixed state. Thus, mechanisms of decoherence, such as the dephasing are the responsible behind the quantum to classical transition. Moreover, as we learn in the bases of statistical mechanics, in the thermal state there is no coherence. Thus, if we are dealing with a thermal process using the tools of quantum mechanics, where we have superpositions into the game, mechanisms of decoherence have an important role in the thermalization. Finally, the contact with a resorvoir causes dephasing and entropy is produced, showing the convergence of the theory of open quantum systems with the expected from the classical thermodynamics.

In the context of fluxes, one-dimensional systems have already been studied classically [24, 25, 26] and quantically [9]. Still in classical mechanics, conservative noises proved to be useful in the process of finding Fourier's law for one-dimensional chains [27]. This motivates us to study the possible effects of conservative noises in quantum systems, still in the context of one-dimensional systems. Thus, in this dissertation we try to understand the role of a conservative noise in the thermalization and entropy production in a bipartite one-dimensional chain, in which each half is prepared in a different thermal state.

This dissertation was divided as follows: in chapter two an introduction to basic concepts of linear algebra and quantum mechanics is made. In chapter three we make an introduction to second quantization, and the grand canonical ensemble, two concepts that will be largely used in the role dissertation. In chapter four we discuss about Onsager reciprocity and fluctuation theorems, giving special attention to the case where there is flux of energy and particles. In chapter five, we discuss the formalism of open quantum systems, starting from the Lindblad master equation until the evolution of averages in open quantum systems and a discussion about decoherence and dephasing noise. In chapter six and seven,the concepts shown previously are applied in the context of the evolution of a bipartite system, with each subsystem prepared at different thermal states, under the influence of a phenomenological dephasing. Finally, chapter seven will have the conclusions and final remarks and certain technical details are left to the appendices.

Chapter 2

Fundamentals of Quantum Mechanics

In this chapter we will summarize the basic concepts of linear algebra and quantum mechanics that will be used in this dissertation [1].

2.1 Linear Algebra for Quantum Mechanics

This section was entirely based on the chapter 2 of the book of Nielsen-Chuang [28]. For readers interested in a more detailed approach, the topics presented here can also be studied in the books of Shankar [29] and Cohen-Tannoudji [30]

The main concepts of linear algebra are the vectors and the vector spaces. The vector space of interest is $\mathcal{C}^n$, which is the space of all set of n complex numbers $(z_1, z_2, ..., z_n)$. The elements of a vector space are called a *vector* and the notation, in a given basis [2], as a column matrix is

$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{pmatrix}. \tag{2.1}$$

The vector spaces have two special properties:

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[1] These introdutory remarks were based on a set of lecture notes of Dr. Jader Pereira dos Santos.

[2] The concept of a basis will be discussed soon.

- The sum between two vectors of the same vector space is also an element of the same vector space.
- The product of a scalar with an element of the vector space is also an element of this space.

In this dissertation, as well as in quantum mechanics, vectors will be denoted as $|\psi\rangle$, where ψ is just a label for the vector.

A basis $\{|v_i\rangle\}$ of a vector space is such that any vector in this space can be written as $\sum_i a_i |v_i\rangle$. For example, for $\mathcal{C}^2$, a possible set is :

$$|v_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |v_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{2.2}$$

because any vector of this space can be written as a linear combination of these.

Usually, a vector space can be written in many different bases. For example, it is also possible to write $\mathcal{C}^2$ using

$$|v_1\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |v_2\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{2.3}$$

It is said that the vectors $|v_1\rangle, ..., |v_n\rangle$ are linearly independent if $\sum_i a_i |v_i\rangle = 0$ if and only if $a_i = 0$ for all i. If this is obeyed, the set $\{|v_i\rangle\}$ is a basis of the vector space V.

2.1.1 Linear Operators and Matrices

A linear operator between two vector spaces V and W is defined as a linear application $A : V \to W$.

$$A\Big(\sum_i a_i |v_i\rangle\Big) = \sum_i a_i A\Big(|v_i\rangle\Big). \tag{2.4}$$

In general we write only $A|v_i\rangle$ to denote $A(|v_i\rangle)$ and we say that a linear operator is defined in the vector space V if $A : V \to V$.

Notation	Description
z^*	Complex conjugate of z
$\|\psi\rangle$	Vector, also called as ket
$\langle\psi\|$	Dual vector of $\|\psi\rangle$, also called as bra
$\langle\phi\|\psi\rangle$	Inner product between $\|\psi\rangle$ and $\|\phi\rangle$
$\|\phi\rangle \otimes \|\psi\rangle$	Tensorial product between $\|\psi\rangle$ and $\|\phi\rangle$
$\|\phi\rangle \|\psi\rangle$	Abbreviated notation of tensor product between $\|\psi\rangle$ and $\|\phi\rangle$
A^*	Complex conjugated of the matrix A
A^T	Transpose of the matrix A
$A^\dagger$	Hermitian conjugated, or adjunt matrix of A, $A^\dagger = (A^T)^*$ $\begin{bmatrix} a & b \\ c & d \end{bmatrix}^\dagger = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$
$\langle\phi\| A \|\psi\rangle$	Scalar product between $\|\phi\rangle$ and $A\|\psi\rangle$ Equivalently, scalar product between $A^\dagger\|\phi\rangle$ e $\|\psi\rangle$

2.1.2 Inner and Outer Products

Given two vectors $|v\rangle$ and $|w\rangle$, the inner product is a function that takes these vectors as entries and gives us a complex number. The notation of inner product in quantum mechanics is

$$\langle v|w\rangle\,, \tag{2.5}$$

where $\langle v|$ is the dual vector of $|v\rangle$, which has the form of a row vector. The inner product obeys the following properties:

$$\begin{aligned} 1)\ \langle v| \left(\sum_i \lambda_i |w_i\rangle \right) &= \sum_i \lambda_i \langle v|w_i\rangle \\ 2)\ \langle v|w\rangle = (\langle w|v\rangle)^* &= \langle w|v\rangle^* \\ 3)\ \langle v|v\rangle \geq 0,\ \ \langle v|v\rangle &\leftrightarrow |v\rangle = 0. \end{aligned}$$

In terms of the components in a basis, the inner product becomes

$$\langle v|w\rangle \equiv \sum_i v_i^* w_i = (v_1^* ... v_n^*) \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}. \tag{2.6}$$

We define the norm of a vector as

$$|| \, |v\rangle \, || \equiv \sqrt{\langle v|v\rangle} \tag{2.7}$$

and when the norm of a vector is one, it is called *unitary vector*. Finally, a set of vectors $\{|i\rangle\}$ is called *orthonormal* if all vectors of this set obey $\langle i|j\rangle = \delta_{ij}$.[3]. In this dissertation, we will always work with orthonormal bases.

We represent linear operators in a so called representation of outer product. Suppose that $|v\rangle$ is a vector of a vector space V and $|w\rangle$ a vector of a vector space W. We then define the linear operator $(|w\rangle \langle v|)$, as a linear operator $V \to W$ whose action on an element of V is given by:

$$\Big(|w\rangle \langle v| \Big) |v'\rangle = |w\rangle \langle v|v'\rangle = \Big(\langle v|v'\rangle \Big) |w\rangle . \tag{2.8}$$

Moreover, we can construct linear combinations like

$$\sum_i a_i |w_i\rangle \langle v_i| \tag{2.9}$$

that acts at $|v'\rangle$ in following way:

$$\left(\sum_i a_i |w_i\rangle \langle v_i| \right) |v'\rangle = \sum_i a_i \Big(\langle v|v'\rangle |w_i\rangle \Big) \tag{2.10}$$

2.1.3 Completeness Relation

Let $\{|i\rangle\}$ be an orthonormal basis of V, such that any vector $|v\rangle$ of this space can be written as $|v\rangle = \sum_i v_i |i\rangle$ for some set of complex numbers v_i. Note that $v_i = \langle i|v\rangle$, and

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[3] $\delta_i j$ is the Kroenecker's delta and has value one for $i = j$ and zero otherwise.

therefore

$$\left(\sum_i |i\rangle \langle i|\right) |v\rangle = \sum_i v_i |i\rangle = |v\rangle\,. \tag{2.11}$$

Such result is valid for any vector $|v\rangle$ and thus

$$\sum_i |i\rangle \langle i| = I \tag{2.12}$$

where I is the identity matrix[4]. This equality is known as *completeness relation.*

One of the usefulness of the completeness relation is writing a certain operator in the representation of outer products. For example, consider a certain operator H and let us multiply it by one twice, using the completeness relation in a basis $\{|i\rangle\}$. Thus we get:

$$H = IHI = \Big(\sum_i |i\rangle \langle i|\Big) H \Big(\sum_j |j\rangle \langle j|\Big). \tag{2.13}$$

Using $H_{ij} = \langle i| H |j\rangle$, the Hamiltonian in the outer product representation is

$$H = \sum_{i,j} H_{ij} |i\rangle \langle j|\,. \tag{2.14}$$

2.1.4 Eigenvalues and Eigenvectors

An *eigenvector* of an operator A in a vector space is a non-null vector $|n\rangle$ such that

$$A|n\rangle = a_n |n\rangle \tag{2.15}$$

where a_n is a complex number called *eigenvalue.* The eigenvalues of an operator A can be found through the secular equation

$$\det|A - a_n I| = 0. \tag{2.16}$$

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[4] Many times in this dissertation, when there is no possibility of ambiguity, I will write 1 instead of I.

The values λ obtained by this equation are the eigenvalues of A. The diagonal representation of an operator A is

$$A = \sum_i \lambda_i \left|i\right\rangle \left\langle i\right| \tag{2.17}$$

such that $\{\left|i\right\rangle\}$ is the set of eigenvectors with the respective eigenvalues λ_i.

2.1.5 Commutator and Anticommutator

The commutator of two operators A and B is defined as

$$[A, B] = AB - BA. \tag{2.18}$$

If $[A, B] = 0$, in other words, $AB = BA$, then we say that A commutes with B and vice-versa. Similarly, the anticommutator of two operators A and B is given by

$$\{A, B\} = AB + BA, \tag{2.19}$$

and if $\{A, B\} = 0$, it is said that A and B anticommute.

2.1.6 Adjoint and Hermitian Operators

The relation between bras e kets allows us to associate each linear operator A with another linear operator, denoted by $A^\dagger$ called adjoint operator (or Hermitian conjugate) of A.

Let $\left|\psi\right\rangle$ be an arbitrary ket belonging to V. The ket $\left|\psi\right\rangle$ is related with $\left\langle\psi\right|$ in the same way that another ket $\left|\psi'\right\rangle$ is related to the bra $\left\langle\psi'\right|$. Then we define $A^\dagger$ as follows:

$$\left|\psi'\right\rangle = A\left|\psi\right\rangle \Leftrightarrow \left\langle\psi'\right| = \left\langle\psi\right| A^\dagger. \tag{2.20}$$

Using scalar product properties, we can see that this definition is consistent because

$$\left\langle\psi'|\phi\right\rangle = \left\langle\psi\right| A^\dagger \left|\phi\right\rangle = \left\langle\phi\right| A \left|\psi\right\rangle = \left\langle\phi|\psi'\right\rangle^* . \tag{2.21}$$

Properties: Consider two linear operators A and B and a complex number λ. The adjoint operation satisfies the following properties:

$$\begin{aligned}(A^\dagger)^\dagger &= A \\ (\lambda A)^\dagger &= \lambda^* A^\dagger \\ (A+B)^\dagger &= A^\dagger + B^\dagger.\end{aligned}$$

We can now compute $(AB)^\dagger$. To do this, let us consider a ket $|\phi\rangle = AB|\psi\rangle$. Writing $|\phi\rangle = A|\chi\rangle$, where $|\chi\rangle = B|\psi\rangle$, we have

$$\langle\phi| = \langle\psi|(AB)^\dagger = \langle\chi|A^\dagger = \langle\psi|B^\dagger A^\dagger \tag{2.22}$$

and therefore

$$(AB)^\dagger = B^\dagger A^\dagger. \tag{2.23}$$

Hermitian Operator: An operator is said to be Hermitian if $A^\dagger = A$.

Unitary Operators: An operator U is said unitary if $U^\dagger U = UU^\dagger = I$. An important property that emerges from this is that

$$(U|v\rangle, U|w\rangle) = \langle v|U^\dagger U|w\rangle = (|v\rangle, |w\rangle), \tag{2.24}$$

and so, we can see that a unitary application does not change the value of the scalar product.

2.1.7 Trace

Trace: The trace of an operator A, written as $\mathrm{tr}(A)$ is the sum of the diagonal elements of A. When we choose a certain basis $\{|i\rangle\}$, we can write

$$\mathrm{tr}(A) = \sum_i \langle i|A|i\rangle. \tag{2.25}$$

Note thar the trace is invariant under change of (orthonormal) basis.

$$\mathrm{tr}(A) = \sum_i \langle i| A |i\rangle = \sum_{i,n} \langle i|n\rangle \langle i| A |n\rangle = \sum_n \langle n| A \Big(\sum_i |i\rangle \langle i| \Big) |n\rangle = \sum_n \langle n| A |n\rangle \tag{2.26}$$

Another important property of the trace is that it is *cyclic*. As an example, consider the trace of an operator product AB:

$$\begin{aligned} \mathrm{tr}(AB) &= \sum_i \langle i| AB |i\rangle = \sum_{i,j} \langle i| A |j\rangle \langle j| B |i\rangle = \sum_{i,j} \langle j| A |i\rangle \langle i| B |j\rangle = \sum_j \langle j| BA |j\rangle \\ &= \mathrm{tr}(BA) \end{aligned} \tag{2.27}$$

If we have a product of three operators, like ABC, it is easy to prove using the same idea that $\mathrm{tr}(ABC) = \mathrm{tr}(CAB) = \mathrm{tr}(BCA)$.

2.2 Postulates of Quantum Mechanics

Here I will introduce the basic postulates of quantum mechanics. This section was entirely based on the book of Cohen [30] and Nielsen and Chuang [28].

Postulate 1: For any isolated physical system, there is an associated complex vector space with inner product (known as a *Hilbert space*), known as space of states of the system. The system is totally described by its state vector, a unitary vector in the space of states.

For example, a two-level system is described in a Hilbert space of dimension 2. Suppose that $|0\rangle$ and $|1\rangle$ constitute an orthonormal basis at this space. An arbitrary vector of this space can be written as

$$|\psi\rangle = a\,|0\rangle + b\,|1\rangle \tag{2.28}$$

where a and b are complex numbers. The unitarity condition says that $\langle\psi|\psi\rangle = 1$, which is equivalent to $|a|^2 + |b|^2 = 1$. This is also called *normalization condition.*

Postulate 2: Each measurable physical quantity is described by an operator. This operator is called an *observable.*

Postulate 3: The possible results of a measurement of an observable A are the eigenvalues of the corresponding observable.

Postulate 4: When an observable is measured in a system described by a normalized state $|\psi\rangle$, the probability $P(a_n)$ of obtaining an eigenvalue a_n of an observable A is

$$P(a_n) = |\langle n|\psi\rangle|^2 \tag{2.29}$$

in which $|n\rangle$ is a normalized eigenstate of A, associated with the eigenvalue a_n. [5]

Postulate 5: The time evolution for a state of a closed quantum system is described by Schrödinger's equation:[6]

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = H |\psi\rangle , \tag{2.30}$$

where $\hbar$ is the reduced Planck's constant and H is the Hamiltonian. In this work, $\hbar$ will be set to one.

2.2.1 Mean Value of an Observable

The mean value of an observable A, given that the state is $|\psi\rangle$ is written as $\langle A\rangle_\psi$ or simply $\langle A\rangle$. If the ket $|\psi\rangle$ is normalized, the mean value $\langle A\rangle$ is given by

$$\langle A\rangle = \langle\psi| A |\psi\rangle . \tag{2.31}$$

Demonstration

Considering that the operator A has discrete spectrum with eigenvalues a_n, the mean value is

$$\langle A\rangle = \sum_n a_n P(a_n) \tag{2.32}$$

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[5] When an eigenvalue is degenerate we have to count all the possibilities that give us the same quantity measured.

[6] ∂_t will sometimes be used to write the derivative in respect to time instead of $\frac{\partial}{\partial t}$.

where $P(a_n)$ is the probability of finding the eigenvalue a_n which is given by $P(a_n) = |\langle n|\psi\rangle|^2 = \langle n|\psi\rangle \langle\psi|n\rangle$. Replacing in eq 2.32, we can write

$$\langle A\rangle = \sum_n a_n \langle n|\psi\rangle \langle\psi|n\rangle = \langle\psi| \Big(\sum_n a_n |n\rangle \langle n| \Big) |\psi\rangle \quad \rightarrow \langle A\rangle = \langle\psi| A |\psi\rangle . \tag{2.33}$$

2.2.2 Solution of Schrödinger's Equation

As we have seen before, for a given vector space, an operator applied to a vector state produces another vector. Consider now Schrödinger's equation, given by the eq. 2.30. If we consider an infinitesimal amount of time variation δt, we can discretize the derivative with respect to time and obtain

$$i\left(\frac{|\psi(t+\delta t)\rangle - |\psi(t)\rangle}{\delta t}\right) = H|\psi(t)\rangle , \qquad \delta t \rightarrow 0 \tag{2.34}$$

and then

$$|\psi(t+\delta t)\rangle = (1 - iH\delta t)|\psi(t)\rangle . \tag{2.35}$$

So, when $(1 - iH\delta t)$ is applied on a ket $|\psi\rangle$, it evolves this ket in an amount of time δt. It shows us the fundamental role of the Hamiltonian in the temporal evolution. We say that the Hamiltonian is the generator of the time evolution.

Now, for any state $|\psi\rangle$ we can use the completeness relation, in order to write this state in some basis $\{|i\rangle\}$. Thus,

$$|\psi\rangle = I|\psi\rangle = \sum_i |i\rangle \langle i|\psi\rangle = \sum_i \psi_i |i\rangle \tag{2.36}$$

in which $\psi_i = \langle i|\psi\rangle$ is a complex number. The normalization condition implies that

$$\langle\psi|\psi\rangle = \sum_i |\psi_i|^2 = 1. \tag{2.37}$$

Back to Schröedinger's equation, applying $\langle i|$ in both sites, we can write

$$\frac{d}{dt}\langle i|\psi\rangle = -i\langle i| H |\psi\rangle = -i\langle i| H\left(\sum_j |j\rangle\langle j|\right)|\psi\rangle \tag{2.38}$$

and then

$$\frac{d}{dt}\psi_i = -iH_{ij}\psi_j, \tag{2.39}$$

which allows us to write Schrödinger's equation in matrix form.

$$\frac{d}{dt}\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\end{pmatrix} = -i\begin{pmatrix}H_{11} & H_{12} & \cdots\\ H_{21} & H_{22} & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\end{pmatrix} \tag{2.40}$$

A very important basis is the one formed by the eigenstates of the Hamiltonian, obtained by solving

$$H\left|n\right\rangle = E_n\left|n\right\rangle \tag{2.41}$$

where E_n are the eigenvalues of H. Using this basis the matrix elements are $\left\langle m\right| H\left|n\right\rangle = \delta_{n,m}E_n$. Using the completeness twice, we write the Hamiltonian as

$$H = \left(\sum_m \left|m\right\rangle\left\langle m\right|\right)H\left(\sum_n \left|n\right\rangle\left\langle n\right|\right) = \sum_n E_n\left|n\right\rangle\left\langle n\right|. \tag{2.42}$$

Then, in the basis of eigenstates of the Hamiltonian, Schrödinger's equation is

$$\frac{d}{dt}\begin{pmatrix}c_1\\ c_2\\ \vdots\end{pmatrix} = -i\begin{pmatrix}E_1 & 0 & \cdots\\ 0 & E_2 & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}c_1\\ c_2\\ \vdots\end{pmatrix} \tag{2.43}$$

in which $c_n(t) = \langle n|\psi(t)\rangle$. Hence

$$\frac{dc_n}{dt} = -iE_nc_n, \quad \rightarrow \quad c_n(t) = c_n(0)e^{-iE_nt} \tag{2.44}$$

where $c_n(0)$ is determited by an initial condition. The ket $\left|\psi(t)\right\rangle$ is reconstructed as

$$\begin{aligned}\left|\psi(t)\right\rangle &= \left(\sum_n \left|n\right\rangle\left\langle n\right|\right)\left|\psi(t)\right\rangle\\ &= \sum_n c_n(0)e^{-iE_nt}\left|n\right\rangle. \end{aligned}\tag{2.45}$$

2.2.3 Time Evolution Operator

We can also solve Schrödinger's equation in a basis independent way:

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle\,, \qquad U(t) = e^{-iHt}. \tag{2.46}$$

The operator $U(t)$ is called *time evolution operator* or *propagator* (because it propagates the state through the time $0 \to t$).

Computing the exponential of an operator, as we can see in the propagator, may be a difficult task, but if one knows the eigenvalues and eigenvectors of the operator, then it is always possible to compute it. To see that, we proceed as follows.

Any element of a power series can be computed as

$$H^j = \sum_n E_n^j\,|n\rangle\,\langle n|\,. \tag{2.47}$$

Then, for a function $f(H)$, which can be expanded in Taylor series, we get:

$$f(H) = \sum_n f(E_n)\,|n\rangle\,\langle n|\,. \tag{2.48}$$

As a direct consequence, in the basis of eigenstates of the Hamiltonian, the propagator is written as

$$e^{-iHt} = \sum_n e^{-iE_n t}\,|n\rangle\,\langle n|\,. \tag{2.49}$$

2.3 Density Matrix

With the purpose of describing a physical system, let us introduce the concept of ensemble. Consider an ensemble as a collection of $\mathcal{N}$ physical systems, identical to each other and prepared at the same macroscopic conditions. The central idea of the theory of ensembles is the expectation of the mean of a certain quantity with respect to the time will be the same obtained by taking the average over the ensemble [31].

Each system of the ensemble is governed by a unique Hamiltonian and the evolution of a certain state is given by Schrödinger's Equation

$$i\partial_t |\psi(t)\rangle = H |\psi(t)\rangle . \tag{2.50}$$

Suppose that $|\alpha, t\rangle$ is a state vector where α is a set of quantum numbers that describes the state of the system completely. If the Hamiltonian is time-independent, then

$$|\alpha, t\rangle = e^{-iHt} |\alpha, 0\rangle = \sum_n e^{-iE_n t} |n\rangle \langle n| \alpha, 0\rangle, \tag{2.51}$$

where we assume that $|n\rangle$ is the set of eigenstates of the Hamiltonian. Considering an operator $\mathcal{O}$, the average over this state is

$$\langle \mathcal{O}(t)\rangle_\alpha \equiv \langle \alpha, t| \mathcal{O} |\alpha, t\rangle . \tag{2.52}$$

Now we can look at the average *over the ensemble*, which will be [31]

$$\langle \mathcal{O}(t)\rangle = \frac{1}{\mathcal{N}} \sum_{ens} \langle \alpha, t| \mathcal{O} |\alpha, t\rangle = \sum_\alpha \frac{N_\alpha}{\mathcal{N}} \langle \alpha, t| \mathcal{O} |\alpha, t\rangle = \sum_\alpha \omega_\alpha \langle \alpha, t| \mathcal{O} |\alpha, t\rangle \tag{2.53}$$

where $\omega_\alpha = N_\alpha/N$ is the probability of the system be in the state α and has to obey the condition $\sum_\alpha \omega_\alpha = 1$.

After this, we can compute the averages using the eigenstate basis of the Hamiltonian. Using

$$|\alpha, t\rangle = \sum_n |n\rangle \langle n| \alpha, t\rangle = \sum_n c_n^\alpha(t) |n\rangle , \tag{2.54}$$

we have

$$\langle \mathcal{O}(t)\rangle = \frac{1}{\mathcal{N}} \sum_{ens} \langle \alpha, t| \mathcal{O} |\alpha, t\rangle = \frac{1}{\mathcal{N}} \sum_{ens} \sum_{n,m} \langle \alpha, t| m\rangle \langle m| \mathcal{O} |n\rangle \langle n| \alpha, t\rangle \tag{2.55}$$

and then

$$\langle O(t)\rangle = \frac{1}{\mathcal{N}} \sum_{n,m} \rho_{nm} \mathcal{O}_{mn} = \mathrm{tr}(\mathcal{O}\rho) \tag{2.56}$$

where

$$\rho_{nm} \equiv \frac{1}{\mathcal{N}} \sum_{ens} \langle n|\alpha, t\rangle \langle \alpha, t|m\rangle = \langle n| \left(\frac{1}{\mathcal{N}} \sum_\alpha N_\alpha |\alpha, t\rangle \langle \alpha, t| \right) |m\rangle . \tag{2.57}$$

Therefore, we are able to define the density matrix ρ as

$$\rho = \sum_{\alpha} \omega_{\alpha} \left|\alpha, t\right\rangle \left\langle\alpha, t\right| . \tag{2.58}$$

Furthermore, a convenient way to express the density matrix is by using the basis of eigenstates. Consider that

$$\rho \left|k\right\rangle = p_k \left|k\right\rangle \tag{2.59}$$

gives us the eigenvalues and eigenvectors. Using this basis we may write the density matrix as

$$\rho = \sum_{k} p_k \left|k\right\rangle \left\langle k\right| . \tag{2.60}$$

2.3.1 Properties of Density Matrix

Here I will present some properties of density matrices, which are discussed in details in [32].

Hermiticity: Using the definition of 2.58 it is clear that

$$\rho = \rho^{\dagger} \tag{2.61}$$

Purity: We say that the system is in a pure state if

$$\rho = \left|\alpha\right\rangle \left\langle\alpha\right| \tag{2.62}$$

which implies

$$\rho^2 = \rho. \tag{2.63}$$

On the other hand, we will call a mixed state those which have more than one p_k different from zero. It implies

$$\rho^2 \neq \rho. \tag{2.64}$$

Trace: The density matrix also has a well defined trace.

$$\mathrm{tr}(\rho) = \sum_{k,k'} p_k \langle k'|\, k\rangle \langle k|\, k'\rangle = \sum_{k'} p_{k'} \langle k'|\, k'\rangle = \sum_{k'} p_{k'} = 1. \tag{2.65}$$

So the trace of a density matrix is also independent of the basis. Another useful quantity is the trace of ρ^2, which is defined as the purity of the system.

$$\mathrm{tr}(\rho^2) = \sum_k p_k^2 \leq 1. \tag{2.66}$$

For a pure ensemble this is trivial because $\rho^2 = \rho$, so that the trace will clearly be the same, but for a mixed ensemble the purity will be smaller than one and consequently, the trace of ρ^2 serves as a measure of the purity of a state.

Positivity: The density matrix is a positive operator, which is written as $\rho \geq 0$. This means that all its eigenvalues are non-negative. To prove this we note that, given eq. 2.58, for an arbitrary state $|\phi\rangle$ we get

$$\langle\phi|\rho|\phi\rangle = \sum_\alpha \omega_\alpha \langle\phi|\alpha, t\rangle \langle\alpha, t|\phi\rangle = \sum_\alpha \omega_\alpha | \langle\alpha, t|\phi\rangle |^2 \tag{2.67}$$

which is clearly non-negative numbers.

When a quadratic form is always non-negative for any state $|\phi\rangle$, it immediately implies that the operator itself must be positive. To see this, simply use $|\phi\rangle$ as an eigenvector $|k\rangle$, which will give $p_k \geq 0$.

2.3.2 Von-Neumann Equation

In order to determine the time evolution of a density matrix in closed quantum systems, let us consider the density matrix $\rho(t_0) = \sum_\alpha w_\alpha |\alpha, t_0\rangle\langle\alpha, t_0|$. As time flows, the states $|\alpha, t_0\rangle$ evolve and consequently the density matrix evolves too. At a given time t, the density matrix is:

$$\rho(t) = \sum_\alpha w_\alpha |\alpha, t\rangle\langle\alpha, t|, \tag{2.68}$$

using the time evolution operator,

$$\begin{aligned} \rho(t) &= \sum_\alpha w_\alpha |\alpha, t\rangle\langle\alpha, t| && (2.69)\\ &= \sum_\alpha w_\alpha U(t,t_0)|\alpha, t_0\rangle\langle\alpha, t_0|U^\dagger(t,t_0) && (2.70)\\ &= U(t,t_0)\left(\sum_\alpha w_\alpha |\alpha, t_0\rangle\langle\alpha, t_0|\right)U^\dagger(t,t_0) && (2.71)\\ &= U(t,t_0)\rho(t_0)U^\dagger(t,t_0). && (2.72) \end{aligned}$$

Differentiating this equation with respect to time, we find:

$$\frac{d\rho(t)}{dt} = -i[H, \rho(t)] \tag{2.73}$$

which is known as *von-Neumman's equation* [33] [7].

2.4 Tensor Products and Reduced Density Matrix

In this section I will discuss the basic ideas and properties of tensor products as well the ones of reduced density matrix. The concepts introduced here will be essential to this dissertation since we shall work extensively with composite systems. [8]

2.4.1 Tensor Products

Imagine that we have two systems A and B with their respectives Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. A tensor product is a way to put these Hilbert spaces [9] together in a bigger one, allowing to describe a composite system $A + B$.

Now, suppose $\mathcal{H}_A$ and $\mathcal{H}_B$ are Hilbert spaces with dimensions m and n, respectively. Then $\mathcal{H}_A \otimes \mathcal{H}_B$ (it reads: $\mathcal{H}_A$ tensor $\mathcal{H}_B$) is a mn dimensional Hilbert space. The elements of $\mathcal{H}_A \otimes \mathcal{H}_B$ are linear combinations of *tensor products* $|a\rangle \otimes |b\rangle$ of elements $|a\rangle$ of $\mathcal{H}_A$ and $|b\rangle$ of

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[7] Sometimes it is called as Liouville - von Neumann's equation, due to its similar form and interpretation, as can be seen in [34]

[8] As great part of this chapter, this section was also based on [28].

[9] It is true not only for Hilbert spaces but also for *any* vector space.

$\mathcal{H}_B$. In particular, if $|\alpha\rangle$ and $|\beta\rangle$ are orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$, then $|\alpha\rangle \otimes |\beta\rangle$, for short $|\alpha\rangle\,|\beta\rangle$ or $|\alpha, \beta\rangle$, is a basis of $\mathcal{H}_A \otimes \mathcal{H}_B$ [28].

Next, I will summarize some properties and consequences of tensor products.

1) For an arbitray scalar z and elements $|a\rangle$ of $\mathcal{H}_A$ and $|b\rangle$ of $\mathcal{H}_B$,

$$z(|a\rangle \otimes |b\rangle) = (z\,|a\rangle) \otimes |b\rangle = |a\rangle \otimes (z\,|b\rangle). \tag{2.74}$$

2) For arbitrary $|a_1\rangle$ and $|a_2\rangle$ of $\mathcal{H}_A$ and $|b\rangle$ of $\mathcal{H}_B$,

$$(|a_1\rangle + |a_2\rangle) \otimes |b\rangle = |a_1\rangle \otimes |b\rangle + |a_2\rangle \otimes |b\rangle\,. \tag{2.75}$$

3) For arbitrary $|b_1\rangle$ and $|b_2\rangle$ of $\mathcal{H}_B$ and $|a\rangle$ of $\mathcal{H}_A$,

$$|a\rangle \otimes (|b_1\rangle + |b_2\rangle) = |a\rangle \otimes |b_1\rangle + |a\rangle \otimes |b_2\rangle\,. \tag{2.76}$$

Still considering the spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ and their bases, let us take an operator $\mathcal{O}^{(A)}$ belonging to $\mathcal{H}_A$ and $\mathcal{O}'^{(B)}$ belonging to $\mathcal{H}_B$. Then we can define a linear operator $\mathcal{O}^{(A)} \otimes \mathcal{O}'^{(B)}$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ by the equation

$$(\mathcal{O}^{(A)} \otimes \mathcal{O}'^{(B)})(|a\rangle \otimes |b\rangle) = (\mathcal{O}^{(A)}\,|a\rangle) \otimes (\mathcal{O}'^{(B)}\,|b\rangle). \tag{2.77}$$

It can also be expanded for linear combinations of tensor products $\sum_i c_i \mathcal{O}_i^{(A)} \otimes \mathcal{O}_i'^{(B)}$ as follows:

$$(\sum_i \mathcal{O}_i^{(A)} \otimes \mathcal{O}_i'^{(B)})\,|a\rangle \otimes |b\rangle = \sum_i \mathcal{O}_i^{(A)}\,|a\rangle\,\mathcal{O}_i'^{(B)}\,|b\rangle\,. \tag{2.78}$$

A convenient, and clearer, way to represent an operator $\mathcal{O}^{(A)} \otimes \mathcal{O}'^{(B)}$ is the matrix representation, known as *Kroenecker product*. Suppose $\mathcal{O}^{(A)}$ is a $m \times n$ matrix and $\mathcal{O}'^{(B)}$ a

$p \times q$ matrix, then in matrix representation, we have

$$\mathcal{O}^{(A)} \otimes \mathcal{O}'^{(B)} = \begin{pmatrix} \mathcal{O}^{(A)}_{11}\mathcal{O}'^{(B)} & \mathcal{O}^{(A)}_{12}\mathcal{O}'^{(B)} & \cdots & \mathcal{O}^{(A)}_{n1}\mathcal{O}'^{(B)} \\ \mathcal{O}^{(A)}_{21}\mathcal{O}'^{(B)} & \mathcal{O}^{(A)}_{22}\mathcal{O}'^{(B)} & \cdots & \mathcal{O}^{(A)}_{n2}\mathcal{O}'^{(B)} \\ \vdots & \vdots & \vdots & \vdots \\ \mathcal{O}^{(A)}_{m1}\mathcal{O}'^{(B)} & \mathcal{O}^{(A)}_{m2}\mathcal{O}'^{(B)} & \cdots & \mathcal{O}^{(A)}_{nm}\mathcal{O}'^{(B)} \end{pmatrix}. \tag{2.79}$$

It is also worth mentioning that this definition also holds for arbitrary rectangular matrices and, in particular, for kets. For instance, consider two vectors $|\alpha\rangle = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ and $|\beta\rangle = \begin{pmatrix} 3 \\ 4 \end{pmatrix}$, then $|\alpha\rangle \otimes |\beta\rangle$ is

$$|\alpha\rangle \otimes |\beta\rangle = \begin{pmatrix} 1\begin{pmatrix} 3 \\ 4 \end{pmatrix} \\ 2\begin{pmatrix} 3 \\ 4 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \\ 6 \\ 8 \end{pmatrix} \tag{2.80}$$

2.4.2 Partial Trace and Reduced Density Matrix

As a motivation of the partial trace, let us first imagine a bipartite system, for simplicity, with identical halves. Suppose that the basis of each part is $\{|i\rangle\}$ and the state of the system is described as

$$|\psi\rangle = \sum_i c_i |i\rangle \otimes |i\rangle . \tag{2.81}$$

Note that if $c_1 = 1$ and the others are zero, then we have a product state. When more than one $c_i \neq 0$, then $|\psi\rangle$ is never a product state and we have an *entangled state*.

Now we want an average of an operator that acts only in the first subsystem, for example

$$\langle A\rangle = \langle\psi| A \otimes I_B |\psi\rangle . \tag{2.82}$$

Using the state defined by eq. 2.81, we find

$$\begin{aligned} \langle A\rangle &= \sum_{i,j} \Big(\langle i| \otimes \langle i| \Big) A \otimes I_B \Big(|j\rangle \otimes |j\rangle \Big) = \sum_{i,j} \langle i| A |j\rangle (\langle i|j\rangle) c_i^* c_j \\ \langle A\rangle &= \sum_i |c_i|^2 \langle i| A |i\rangle . \end{aligned} \tag{2.83}$$

We therefore see from this result that, from the perspective of system A, we can write the expectation value of an operator as an expectation value over a mixed state, described by the density matrix

$$\rho_A = \sum_i |c_i|^2 |i\rangle\langle i| \tag{2.84}$$

Now, let us consider an operator that acts over the two systems.

$$\mathcal{O} = A \otimes B, \quad |a, b\rangle = |a\rangle \otimes |b\rangle \tag{2.85}$$

Then, the average of $\mathcal{O}$ is

$$\langle \mathcal{O} \rangle = \sum_{a,b} \langle a| \otimes \langle b| \, A \otimes B \, |a\rangle \otimes |b\rangle = \sum_a \langle a| \, A \, |a\rangle \otimes \sum_b \langle b| \, B \, |b\rangle = \mathrm{tr}(A)\mathrm{tr}(B). \tag{2.86}$$

Therefore, we can conclude that

$$\mathrm{tr}(A \otimes B) = \mathrm{tr}(A)\mathrm{tr}(B). \tag{2.87}$$

We can also imagine an operation that traces only a part of the system. This operation is called *partial trace* and is defined as

$$\mathrm{tr}_A(A \otimes B) = \mathrm{tr}(A) B \tag{2.88}$$

$$\mathrm{tr}_B(A \otimes B) = \mathrm{tr}(B) A \tag{2.89}$$

$$. \tag{2.90}$$

Note that the result of a partial trace is an operator. For a general operator $\mathcal{O} = \sum_i A_i \otimes B_i$ we have

$$\mathrm{tr}_A(\mathcal{O}) = \sum_i \mathrm{tr}(A_i) B_i \tag{2.91}$$

$$\mathrm{tr}_B(\mathcal{O}) = \sum_i \mathrm{tr}(B_i) A_i \tag{2.92}$$

Let us now return to the original proposition, with a state $\rho_{AB} = |\psi\rangle\langle\psi|$, where $|\psi\rangle$ is given by Eq.(2.81). In this case, applying eq.(2.91) we immediately recover the previous result

Eq.(2.84)

2.5 Interaction Picture

Many problems in quantum mechanics are not exactly soluble. Thus approximative techniques play an important role in the process of obtaining analytical solutions. One of the most important is the approach of the *interaction picture*[35], which will be discussed in this section.

So, we begin considering a Hamiltonian of the form

$$H = H_0 + V. \tag{2.93}$$

Here, H_0 is a diagonalizable Hamiltonian and V is a perturbation, that in applications of interaction picture is typically small compared to H_0.

As discussed in section 2.3, the mean value of an operator $\mathcal{O}$ is given by:

$$\langle \mathcal{O}(t) \rangle = \mathrm{tr}[\mathcal{O}(t)\rho(t)]. \tag{2.94}$$

Inserting some identities, we find

$$\langle \mathcal{O}(t) \rangle = \mathrm{tr}[e^{iH_0 t}\mathcal{O}e^{-iH_0 t}e^{iH_0 t}\rho(t)e^{-iH_0 t}]. \tag{2.95}$$

These results motivate us to introduce the interaction picture form for operators :

$$\mathcal{O}_I(t) = e^{iH_0 t}\mathcal{O}(t)e^{-iH_0 t} \tag{2.96}$$

$$\rho_I(t) = e^{iH_0 t}\rho(t)e^{-iH_0 t} \tag{2.97}$$

Using these definitions, we see that:

$$\langle \mathcal{O}(t) \rangle = \mathrm{tr}[\mathcal{O}_I\rho_I(t)]. \tag{2.98}$$

Now we go ahead and determine the time evolution of $\rho_I(t)$. Let us start remembering the von-Neumann equation in the Schödinger picture

$$\frac{d\rho(t)}{dt} = -i[H, \rho(t)]. \tag{2.99}$$

Then we take the definition of $\rho_I(t)$ and take the derivative with respect to time and one finds

$$\begin{aligned}\frac{d\rho_I(t)}{dt} &= iH_0 e^{iH_0 t}\rho(t)e^{-iH_0 t} + e^{iH_0 t}\frac{d\rho(t)}{dt}e^{-iH_0 t} + e^{iH_0 t}\rho(t)e^{-iH_0 t}(-iH_0) \\ &= i[H_0, \rho_I(t)] + e^{iH_0 t}\frac{d\rho(t)}{dt}e^{-iH_0 t} \\ &= i[H_0, \rho_I(t)] - ie^{iH_0 t} i[H_0 + V, \rho_I(t)]e^{-iH_0 t}\end{aligned} \tag{2.100}$$

and thus

$$\begin{aligned}\frac{d\rho_I(t)}{dt} &= -ie^{iH_0 t}(V_I\rho(t) - \rho(t)V_I)e^{-iH_0 t} \\ &= -i(e^{iH_0 t}Ve^{-iH_0 t}e^{iH_0 t}\rho(t)e^{-iH_0 t} + e^{iH_0 t}\rho(t)e^{-iH_0 t}e^{iH_0 t}Ve^{-iH_0 t})\end{aligned} \tag{2.101}$$

and finally

$$\frac{d\rho_I(t)}{dt} = -i[V_I(t), \rho_I(t)], \tag{2.102}$$

where $V_I(t) \equiv e^{iH_0 t}Ve^{-iH_0 t}e^{iH_0 t}$. Therefore, the time evolution of the density matrix in the interaction picture depends only on the potential written in this representation.

2.6 Entropy and Mutual Information

The concept of entropy plays a central role in statistical mechanics due to its connection with thermodynamics and information theory. For example, if we take a cube of ice and put it on the floor on a sunny day we will see the ice liquify. In terms of quantity of energy and the first law of thermodynamics, nothing prevents us from having the inverse process, but we do not see water solidifying spontaneously on a sunny day. It occurs because the process of liquifying the ice maximizes the entropy and the inverse process minimizes the entropy. Moreover, the laws of physics are the same, independently of the instant that one is looking. So, if we take two photos of the sunny day, one showing the ice cube and the other showing the liquid water, we will immediately know that the photo of the ice was taken before. Therefore, entropy is also the essential quantity giving rise to the arrow of time and the notion of irreversibility. .

The von Neumann entropy provides an approach to quantum statistical mechanics and thermodynamics and it is defined as

$$S(\rho) \equiv -\mathrm{tr}\{\rho \ln(\rho)\}, \quad k_B = 1. \tag{2.103}$$

Using the spectral decomposition of the density matrix

$$\rho = \sum_k p_k \left|k\right\rangle \left\langle k\right| \tag{2.104}$$

allow us to write S as

$$S(\rho) = -\sum_k p_k \ln p_k. \tag{2.105}$$

A statistical mixture which is described by ρ can be obtained mixing pure ensembles described by $|k\rangle$ with corresponding weights p_k. Then $S(\rho)$ expresses our lack of knowledge of the realization of a particular state $|k\rangle$ in the mixture.

Properties:

1: $S(\rho) \geq 0$

The non-negativity of the entropy can be analyzed by writing eq.2.105 as

$$S(\rho) = \sum_k p_k \ln\left(\frac{1}{p_k}\right). \tag{2.106}$$

Knowing that $0 \leq p_k \leq 1$ and $0 \leq \ln\left(\frac{1}{p_k}\right) < \infty$, then it is clear that $p_k \ln(\frac{1}{p_k})$ is non negative and, hence, so is the entropy.

2: If the dimension $\mathcal{D}$ of the Hilbert space is finite, $S(\rho)$ will be bounded from above:

$$S(\rho) \leq \ln \mathcal{D}. \tag{2.107}$$

The equality occurs when the mixture is maximum. In this case, $\rho = \frac{1}{\mathcal{D}}$ and all probabilities p_k will also be $\frac{1}{\mathcal{D}}$.

3 Consider a composite system with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Let ρ_{AB} denote the total density matrix of the system and ρ_A, ρ_B the corresponding reduced density matrices. Then the von Neumann entropy obeys the so called subadditivity condition:

$$S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B), \tag{2.108}$$

where the equality holds for $\rho_{AB} = \rho_A \otimes \rho_B$. The joint entropy measures our total lack of information about a composite system [28].

Eq. (2.108) is the starting point for quantifying the degree of correlation between two systems by means of the *mutual information.*. In other words, how much correlated they are in a sense that how much knowing about one of these systems reduces the uncertainty about the other system. For instance, if two systems A and B are independent, then knowing A does not give us any information about B and vice versa, so their mutual information is null. The mutual information as a function of the individual entropies and the total entropy and is defined by [36]

$$\mathcal{I} \equiv S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \tag{2.109}$$

Clearly, from Eq. (2.113) we see that $\mathcal{I}$ is always non-negative, being zero if and only if ρ_{AB} is a product state, in which case A and B are uncorrelated. The concept of mutual information can be expanded for multipartite systems as discussed in [37]. For the purpose of this dissertation, we will pay atention only for the mutual information for bipartite systems. The mutual information may also be written in terms of the relative entropy :

$$\mathcal{I} = S(\rho_{AB}||\rho_A \otimes \rho_B), \tag{2.110}$$

where

$$S(\rho_{AB}||\rho_A \otimes \rho_B) = \mathrm{tr}\{\rho_{AB}(\ln \rho_{AB} - \ln \rho_A \otimes \rho_B)\} \tag{2.111}$$

which is usually interpreted as a distance between two states.[10]

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[10] One may note, notwithstanding, that the relative entropy is not a proper measure of distance, as it is not symmetric and does not satisfy the triangle inequality

Chapter 3

Second Quantization and Basic Statistical Mechanics

In this chapter I will discuss the fundamental ideas and techniques used in this dissertation, such as how to work with second quantization, which was entirely based on [38, 39], the idea of the tight binding model and how to diagonalize tight-binding Hamiltonians, which were based on [40, 41, 42]. Finally, the chapter is finished with a discussion about basics ideias of the grand canonical ensemble, which was based on [43, 44] .

3.1 Introduction to Second Quantization

Historically, quantum physics first dealt only with the quantization of particles, leaving the eletromagnetic field classical and hence the name quantum mechanics. Later, also the eletromagnetic field was quantized and even particles got represented by quantized fields, resulting in the so called quantum field theory. By convention, the original formulation is called *first quantization*, while quantum field theory and many-body particles physics are written in the language of *second quantization* [45].

In this section, we will construct the basic ideias of second quantization. Here I will not be very rigorous but I will try to construct the theory using intuitive concepts. The basic elements of this theory are the creation and annihilation operators and with them we are able to describe systems interacting with a potential or particles interacting with each other. Then, imagine a system with $\mathcal{N}$ particles of Hamiltonian H whose eigenstates $|n_{\nu_1}, n_{\nu_2}, n_{\nu_3}, ...\rangle$, where n_{ν_i} are limited by $\sum_i n_{\nu_i} = \mathcal{N}$, describe fully the state of the system, where ν_i are the states in which a particle can be and $i = 1, 2, 3, \cdots, N$ is the number of states that can be occupied.

In order to describe a system with one or more particles,we first define the vacuum state which is usually written as $|0\rangle$. With this at hand, one is able to construct the possible states using creation operators. The operation of the creation operator of a particle in some state ν_i, denoted as $a^\dagger_{\nu_i}$, is defined as:

$$a^\dagger_{\nu_i} |0\rangle = |1_{\nu_i}\rangle . \tag{3.1}$$

On the other hand, one may start with some state $|1_{\nu_i}\rangle$ and want to annihilate a particle. For this we define the annihilation operator, that operates in the following way:

$$a_{\nu_i} |1_{\nu_i}\rangle = |0\rangle . \tag{3.2}$$

The next possible step is to describe multi-particle states. As follows, I will construct a two-particle state. Once again we start from the vacuum but now we will operate with $a^\dagger_{\nu_i} a^\dagger_{\nu_j}$:

$$a^\dagger_{\nu_i} a^\dagger_{\nu_j} |0\rangle = a^\dagger_{\nu_i} |1_{\nu_j}\rangle = |1_{\nu_i}, 1_{\nu_j}\rangle \tag{3.3}$$

Let us take some care now. So far I have said nothing about the type of particle, if they were fermions or bosons, I was just creating or destroying one particle. Indeed for one particle states we have no problems, but for many-particle systems it is necessary to consider the symmetrization and antisymmetrization of the states. Fermionic states are antisymmetric and bosonic states are symmetric. So for bosons

$$|1_{\nu_i}, 1_{\nu_j}\rangle = |1_{\nu_j}, 1_{\nu_i}\rangle \tag{3.4}$$

and therefore,

$$a^\dagger_{\nu_i} a^\dagger_{\nu_j} |0\rangle = a^\dagger_{\nu_j} a^\dagger_{\nu_i} |0\rangle . \tag{3.5}$$

Comparing both sides, it is clear that

$$a^\dagger_{\nu_i} a^\dagger_{\nu_j} = a^\dagger_{\nu_j} a^\dagger_{\nu_i} \tag{3.6}$$

and consequently,

$$[a^\dagger_{\nu_i}, a^\dagger_{\nu_j}] = 0. \tag{3.7}$$

Moreover, we are also able to see that $a^\dagger_{\nu_i}$ do not commute with a_{ν_i} just seeing that

$$a^\dagger_{\nu_i} a_{\nu_i} |0\rangle = 0, \qquad a_{\nu_i} a^\dagger_{\nu_i} |0\rangle = |0\rangle \tag{3.8}$$

and therefore [1]

$$[a_{\nu_i}, a^\dagger_{\nu_i}] |0\rangle = |0\rangle \ \rightarrow \ [a_{\nu_i}, a^\dagger_{\nu_i}] = 1 \tag{3.9}$$

For bosons, we can also construct a system with many particles at the same state. I will denote $|n_{\nu_i}\rangle$ a system with n particles at the state ν_i. Moreover, a state $|n_{\nu_i}, m_{\nu_j}\rangle$ means that we have a system with n particles in the state ν_i and m in the state ν_j. So to construct a generic many-particle state, we only need a label to identify the state and the number of particles in it. Sometimes, in order to simplify the notation, we define an order of each state and write it only with the occupation in each one. For example

$$|1_{\nu_1}, 2_{\nu_2}, 0_{\nu_3}, ...\rangle \text{ can be written as } |1, 2, 0, ...\rangle \tag{3.10}$$

and one will know that the system has one particle in the state ν_1, two in ν_2 and zero in ν_3.

Albeit a_{ν_i} is not a hermitian operator, we can construct a hermitian operator using a_{ν_i} and $a^\dagger_{\nu_i}$ with the interpretation of a *number operator*. Let us consider an operator $a^\dagger_{\nu_i} a_{\nu_i}$:

$$[a^\dagger_{\nu_i} a_{\nu_i}, a_{\nu_i}] = a^\dagger_{\nu_i} a_{\nu_i} a_{\nu_i} - a_{\nu_i} a^\dagger_{\nu_i} a_{\nu_i} = -a_{\nu_i} \tag{3.11}$$

and

$$[a^\dagger_{\nu_i} a_{\nu_i}, a^\dagger_{\nu_i}] = a^\dagger_{\nu_i} a_{\nu_i} a^\dagger_{\nu_i} - a^\dagger_{\nu_i} a^\dagger_{\nu_i} a_{\nu_i} = a^\dagger_{\nu_i}. \tag{3.12}$$

---

[1] We can also use this ideia to prove that creation and destruction operators of different states ν will also commute.

Now, let $|\phi\rangle$ be an eigenstate of $a^\dagger_{\nu_i} a_{\nu_i}$ such that $a^\dagger_{\nu_i} a_{\nu_i} |\phi\rangle = \lambda |\phi\rangle$. The first result from this is

$$\langle\phi| a^\dagger_{\nu_i} a_{\nu_i} |\phi\rangle = |a_{\nu_i} |\phi\rangle|^2 \geq 0 \tag{3.13}$$

and therefore $\lambda \geq 0$. Now, we go further and analyze the following cases:

$$(a^\dagger_{\nu_i} a_{\nu_i}) a_{\nu_i} |\phi\rangle = (a_{\nu_i} a^\dagger_{\nu_i} - 1) a_{\nu_i} |\phi\rangle = (\lambda - 1) a_{\nu_i} |\phi\rangle . \tag{3.14}$$

So, if $|\phi\rangle$ is an eigenstate of $a^\dagger_{\nu_i} a_{\nu_i}$, then $a_{\nu_i} |\phi\rangle$ is also an eigenstate of it, but with reduced eigenvalue $\lambda - 1$. Thanks to the condition $\lambda \geq 0$ and the application of a_{ν_i} on a certain state, we conclude that $\lambda = 0, 1, 2, ...$ and just using $|\phi\rangle = |n_{\nu_i}\rangle$, we find

$$a^\dagger_{\nu_i} a_{\nu_i} |n_{\nu_i}\rangle = n |n_{\nu_i}\rangle . \tag{3.15}$$

Moreover, we are also able to see that $a^\dagger_{\nu_i} |n_{\nu_i}\rangle \propto |(n+1)_{\nu_i}\rangle$. Using the same idea used with a_{ν_i}, we have

$$a^\dagger_{\nu_i} a_{\nu_i} a^\dagger_{\nu_i} |n_{\nu_i}\rangle = (n+1) a^\dagger_{\nu_i} |n_{\nu_i}\rangle . \tag{3.16}$$

Through the normalization of the states, we obtain

$$a_{\nu_i} |n_{\nu_i}\rangle = \sqrt{n} |(n-1)_{\nu_i}\rangle \tag{3.17}$$

and

$$a^\dagger_{\nu_i} |n_{\nu_i}\rangle = \sqrt{n+1} |(n+1)_{\nu_i}\rangle \tag{3.18}$$

Next we turn to the case of Fermions. We start using the antisymmetrization of exchanged particles states, which reads:

$$|\nu_i, \nu_j\rangle = - |\nu_j, \nu_i\rangle \tag{3.19}$$

and therefore

$$a^\dagger_{\nu_i} a^\dagger_{\nu_j} |0\rangle = -a^\dagger_{\nu_j} a^\dagger_{\nu_i} |0\rangle . \tag{3.20}$$

Comparing both sides we conclude that

$$a^\dagger_{\nu_i} a^\dagger_{\nu_j} = -a^\dagger_{\nu_j} a^\dagger_{\nu_i}. \tag{3.21}$$

so,

$$\{a^\dagger_{\nu_i}, a^\dagger_{\nu_j}\} = 0, \tag{3.22}$$

which also implies [2]

$$a^\dagger_{\nu_i} a^\dagger_{\nu_i} = -a^\dagger_{\nu_i} a^\dagger_{\nu_i} \to a^\dagger_{\nu_i} a^\dagger_{\nu_i} = 0 \tag{3.23}$$

In other words, fermions have restrictions concerning the creation of states. This restriction is called "Pauli's Principle of Exclusion". We can now describe a many-particle state only with the occupation as we did for bosons, for instance, the ket $|1_{\nu_1}, 0_{\nu_2}, 1_{\nu_3}, ...\rangle = |1, 0, 1, ...\rangle$. One may also see that:

$$(a^\dagger_{\nu_j} a_{\nu_j})^2 = a^\dagger_{\nu_j} a_{\nu_j}(1 - a_{\nu_j} a^\dagger_{\nu_j}) = a^\dagger_{\nu_j} a_{\nu_j}. \tag{3.24}$$

This implies that the eigenvalues of the operator $a^\dagger_{\nu_j} a_{\nu_i}$ is only zero or one, as we saw before.

With this construction, we now have the tools to create and destroy particles as well as we have on hands operators that count the number of particles at a give state. Now we can go further and construct other operators based on creation and annihilation operators. First, consider the single particle states $|\nu_i\rangle$ that are the set of eigenstates of some operator $\mathcal{O}$ with eigenvalues λ_i, related to an additive [3] quantity, such as momentum or kinectic energy.

For a multiparticle state

$$|\psi\rangle = |\nu_1, \nu_2, ...\rangle \tag{3.25}$$

we expect that the eigenvalues of the multiparticle operators $\mathcal{O}$ to be $\sum_i \lambda_i n_{\nu_i}$. It becomes easier to see if we write

$$\mathcal{O} = \sum_i \lambda_i a^\dagger_{\nu_i} a_{\nu_i}. \tag{3.26}$$

Now, suppose that we began in another basis, and for this, let us write $|\nu_i\rangle = \sum_j |\mu_j\rangle \langle\mu_j|\nu_i\rangle$.

---

[2] It is clear that if you can not create two particles at the same state, you can not destroy two particle at the same state as well.

[3] An additive quantity $A(k)$ is such that $A(\lambda k) = \lambda A(k)$, in which λ is a number.

Then, defining $b_j^\dagger$ by the creation $b_j^\dagger |0\rangle = |\mu_j\rangle$, we find

$$a_i^\dagger = \sum_j b_j^\dagger \langle \mu_j | \nu_i \rangle \,, \qquad a_i = \sum_j \langle \nu_i | \mu_j \rangle \, b_j. \tag{3.27}$$

Thus, we can write $\mathcal{O}$ as

$$\begin{aligned} \mathcal{O} &= \sum_i \lambda_i a_{\nu_j}^\dagger a_{\nu_i} = \sum_i \lambda_i \sum_{n,m} b_n^\dagger \langle \mu_n | \nu_i \rangle \langle \nu_i | \mu_m \rangle \, b_m \\ &= \sum_{n,m} b_n^\dagger b_m \sum_i \langle \mu_n | \nu_i \rangle \, \lambda_i \, \langle \nu_i | \mu_m \rangle \\ &= \sum_{n,m} b_n^\dagger b_m \, \langle \mu_n | \mathcal{O} | \mu_m \rangle \\ \mathcal{O} &= \sum_{m,n} \mathcal{O}_{nm} b_n^\dagger b_m. \end{aligned} \tag{3.28}$$

This is the general form of an operator related to an additive quantity using second quantization. In general, we will have in the beginning the form above in which the task will be to diagonalize $\mathcal{O}$, that will give us the eigenvalues.

Other types of operators can be constructed using the second quantization. Terms of potentials and scattering can be written as a linear combination of quartic terms. As we will not use them in this dissertation, I will not make explicit the shape of such interactions. [4]

3.2 Tight binding model

In the beginning of the first course of quantum mechanics, one of the first things that we learn in our classes is to obtain the possible energies of a system, by finding the eigenvalues of Schrödinger's equation. For more complicated systems, finding the energies or the eigenstates may not be an exactly accomplishable task. Thus, for multi-particle or more complicated systems, it is necessary to have on hands some approximation methods.

In solid state physics, there are some methods to calculate approximately these possible energies or states. For example, for a periodic solid one is able to use the *celular method*, where instead of solving for the full solid, we just solve for the unit that will be repeated. Another popular technique is the tight binding model, which will be discussed in this section.

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[4] For a detailed account, see *Modern Quantum Mechanics*, of Sakurai et al.

To understand the ideia of the tight binding model, consider a lattice with N sites and in each one there is one proton and then one puts an electron in any site. The bound states formed can be approximated as hydrogen atom states. Now, to know in what state the electron is, it is necessary to know in what site n and the orbital, let us call μ, that the electron is. Once there is one proton per site, we can consider a periodic electrical potential through the lattice. Thus the electron has a probability to jump from one site to another through the lattice and from one state μ to an μ'. We also expect that the electron will tunnel through one barrier of his site to the next. In other words, we a priori expect that the transition will be like $(n, \mu) \rightarrow (n \pm 1, \mu')$.

Next we think about the change of orbitals $\mu \rightarrow \mu'$. It is clear that if the electron changes the level, considering the hydrogen levels, it will have some cost of energy. Hence, it is more likely that the electron tunnels through the lattice staying in orbitals of the same energy because the cost of transition will be null.

So, a priori, the Hamiltonian of exchange of sites will be:

$$H = \sum_{\mu,\mu'} \sum_{n} t_{\mu,\mu',n} (a^{\dagger}_{n+1,\mu'} a_{n,\mu} + a^{\dagger}_{n,\mu} a_{n+1,\mu'}), \tag{3.29}$$

and after neglecting inter-orbital transitions we get

$$H = \sum_{\mu} \sum_{n} t_{\mu,n} (a^{\dagger}_{n+1,\mu} a_{n,\mu} + a^{\dagger}_{n,\mu} a_{n+1,\mu}). \tag{3.30}$$

This is the so called *tight binding Hamiltonian* and is used extensively to compute the energy band of solids, such as graphene [46, 47, 48, 49, 50, 51, 52].

This Hamiltonian describes the ideia of change of site, for example, the term $a^{\dagger}_{n+1} a_n$ tells us that one particle in the site n is being destroyed and one particle is being created in the next site.

Once the orbitals μ and μ' are uncorrelated by this approach, then we can choose one specific orbital of interest and analyze it separately. So we can drop out the indice μ and the Hamiltonian will be:

$$H = \sum_{n} t_n (a^{\dagger}_{n+1} a_n + a^{\dagger}_n a_{n+1}). \tag{3.31}$$

The ideia of the tight-binding is also applicable in two or three dimensional cases. We have opted to limit our discussion to the one-dimensional case, as this will be the situation of interest in this dissertation.

3.2.1 Two Site Problem

With the goal of understanding the idea of these techniques, let us first imagine a simple problem. Imagine a system composed of 2 sites. If we are dealing with bosons, there is no problem to have more than one particle per site, but for fermions, the Pauli's Exclusion Principle has to be taken into account. Let us consider obeying the tight binding model. For two sites, taking for practicity $t_n = \alpha$, the Hamiltonian can be expressed as:

$$H = \alpha(a_1^\dagger a_2 + a_2^\dagger a_1). \tag{3.32}$$

The solution of the eigenvalue equation in this case is not directly clear, but the idea is to find a transformation that makes the Hamiltonian diagonal. Thus the objective is to put the Hamiltonian in the following form:

$$H = \epsilon_1 b_1^\dagger b_1 + \epsilon_2 b_2^\dagger b_2. \tag{3.33}$$

Once this system is reasonably simple, we may make the following explicit ansatz:

$$a_1 = \frac{b_1 + b_2}{\sqrt{2}} \qquad a_2 = \frac{b_1 - b_2}{\sqrt{2}}. \tag{3.34}$$

We are now able to compute the terms in the Hamiltonian:

$$a_1^\dagger a_2 = \frac{1}{2}(b_1^\dagger + b_2^\dagger)(b_1 - b_2) = \frac{1}{2}(b_1^\dagger b_1 - b_1^\dagger b_2 + b_2^\dagger b_1 - b_2^\dagger b_2) \tag{3.35}$$

$$a_2^\dagger a_1 = \frac{1}{2}(b_1^\dagger - b_2^\dagger)(b_1 + b_2) = \frac{1}{2}(b_1^\dagger b_1 + b_1^\dagger b_2 - b_2^\dagger b_1 - b_2^\dagger b_2) \tag{3.36}$$

Replacing these two results in the original Hamiltonian, we get:

$$H = \alpha(b_1^\dagger b_1 - b_2^\dagger b_2) \qquad \epsilon_1 = \alpha \qquad \epsilon_2 = -\alpha. \tag{3.37}$$

With this simple ansatz, the Hamiltonian is therefore put in diagonal form . However, we have a point to discuss: we put a factor of $\sqrt{2}$ in Eq.(3.34). This term emerges from the fact that we want the same commutations and anticommutations relations, which means, if we start working with fermionic operators, the new set will also be fermionic. The same is also valid for bosonic operators. In other words, if $[a_i, a_j^\dagger] = \delta_{ij}$, then $[b_i, b_j^\dagger] = \delta_{ij}$ for bosons and $\{a_i, a_j^\dagger\} = \delta_{ij}$, then $\{b_i, b_j^\dagger\} = \delta_{ij}$ for fermions.

This makes our transformation matrix unitary.

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{3.38}$$

In other words:

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = S \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{3.39}$$

where

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{3.40}$$

is the transformation matrix in question.

3.3 One dimentional chain

Now let us consider a system formed by N sites, organized as a one-dimensional chain as shown in Fig.(3.1). We shall model the Hamiltonian as:

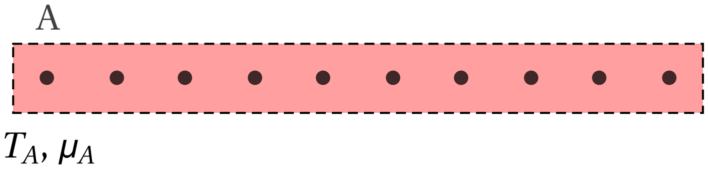

Figure 3.1: A homogeneous chain with 10 sites.

$$H = -\alpha \sum_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) \tag{3.41}$$

Here the operators $a_i^\dagger$ and a_i are the creation and destruction operators referring to the site i as discussed before.

3.3.1 Diagonalizing the Hamiltonian

It is possible to write any quadratic (in the creation and annihilation operators) Hamiltonian as follows:

$$H = \sum_{i,j} W_{ij} a_i^\dagger a_j \tag{3.42}$$

The case of Eq. (3.41), for instance, corresponds to the tri-diagonal matrix. We want to solve $H|\psi\rangle = E|\psi\rangle$ and for this, we have a group of techniques for this task.

There are two forms to treat a $1D$ chain, the first one called *open boundary conditions*, which is an open chain, as it can be seen in the figure 3.1. The other form is called *periodic boundary conditions*, which is a circle formed by the junction of the first and the last sites.

The matricial form of W explicitly is

$$W = \begin{pmatrix} 0 & -\alpha & 0 & 0 & \dots & 0 & 0 & -\alpha \\ -\alpha & 0 & -\alpha & 0 & \dots & 0 & 0 & 0 \\ 0 & -\alpha & 0 & -\alpha & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -\alpha & 0 & 0 & 0 & \dots & 0 & -\alpha & 0 \end{pmatrix} \tag{3.43}$$

for the periodic boundary conditions and,

$$W = \begin{pmatrix} 0 & -\alpha & 0 & 0 & \dots & 0 & 0 & 0 \\ -\alpha & 0 & -\alpha & 0 & \dots & 0 & 0 & 0 \\ 0 & -\alpha & 0 & -\alpha & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & -\alpha & 0 \end{pmatrix} \tag{3.44}$$

for the open chain.

Previously, we made an ansatz in order to obtain a sum of $b_k^\dagger b_k$ to solve that problem. Now we want a general solution for our Hamiltonian.

Based on our previous discussion, let us write our Hamiltonian as a sum of operators $b_k^\dagger b_k$:

$$H = \sum_k \epsilon(k) b_k^\dagger b_k \tag{3.45}$$

where $\epsilon(k)$ [5] are the eigenvalues of the matrix W.

The matrix W must be Hermitian since H must be a Hermitian operator. Hence, we may write it as

$$W = S\Lambda S^T \tag{3.46}$$

where S is a matrix built with its columns being eigenvectors of W and Λ a diagonal matrix where the non-null values are the eigenvalues of W.

Now it is possible to use this form of W to rewrite the Hamiltonian. The element of the matrix W_{ij} is:

$$W_{ij} = \sum_k S_{ik}(\Lambda S^T)_{kj} = \sum_k S_{ik}\Lambda_{kl}S^T_{lj} \tag{3.47}$$

Λ is a diagonal matrix, so

$$\Lambda_{kl} = \Lambda_k \delta_{kl}, \tag{3.48}$$

and then,

$$W_{ij} = \sum_k S_{ik}\Lambda_k S^T_{kl}. \tag{3.49}$$

Replacing this result in the Hamiltonian, we obtain:

$$H = \sum_{ij}\Big(\sum_k S_{ik}\Lambda_k S^T_{kl}\Big)a_i^\dagger a_j = \sum_k \Lambda_k\Big[\sum_i S_{ik}a_i^\dagger\Big]\Big[\sum_j S_{jk}a_j\Big] \tag{3.50}$$

By comparison, we find

$$b_k = \sum_i S_{ik}a_j. \tag{3.51}$$

3.3.2 Solving for a full chain

We discussed that W can assume two forms, depending if one wants to work with periodic boundary conditions or not. Here we will solve both cases.

---

[5] Sometimes, for simplicity, I will write $\epsilon(k)$ as ϵ_k

I-Periodic Boundary Conditions: The first case to be treated is the one with periodic boundary conditions. The shape of the Hamiltonian suffers no changes, except the boundary terms, so this system is also described by Eq.(3.41).

In the case of two sites, we were able to do a simple ansatz that diagonalized the Hamiltonian. To diagonalize in this case we do another ansatz. Recognizing the translational simmetry, one can use the Fourier's transformation as ansatz [6]:

$$a_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ikx_i} b_k^\dagger, \qquad x_i = i. \tag{3.52}$$

Moreover, note that in this dissertation will always consider a unitary lattice spacing .

Even though the particle number operator does not appear directly in the Hamiltonian, it is interesting to see that our transformation does not change the number of particles. The total number of particles, written as $\sum\limits_i a_i^\dagger a_i$, is transformed as follows:

$$a_i^\dagger a_i = \frac{1}{N} \sum_{k,k'} e^{ix_i(k-k')} b_k^\dagger b_k \tag{3.53}$$

and then

$$\sum_i a_i^\dagger a_i = \left(\frac{1}{N} \sum_i e^{ix_i(k-k')} \right) \sum_{k,k'} b_{k'}^\dagger b_k \tag{3.54}$$

The first parenthesis is, by definition, $\delta_{k,k'}$. So, when we apply this Kroenecker's Delta at the double sum, we get:

$$\sum_i a_i^\dagger a_i = \sum_k b_k^\dagger b_k. \tag{3.55}$$

Now we look at the terms of exchange contained in the Hamiltonian $a_{i+1}^\dagger a_i$ and $a_i^\dagger a_{i+1}$

$$a_i^\dagger a_{i+1} = \frac{1}{N} \Big[\sum_k e^{ikx_i} b_k^\dagger \Big] \Big[\sum_{k'} e^{-ik(x_i+1)} b_k^\dagger \Big] = \frac{1}{N} \sum_{k,k'} e^{ix_i(k-k')} = \sum_{k,k'} b_k^\dagger b_{k'} e^{-ik'} \sum_i \frac{1}{N} e^{ix_i(k-k')} \tag{3.56}$$

Therefore,

$$\sum a_i^\dagger a_{i+1} = \sum_k e^{-ik} b_k^\dagger b_k \tag{3.57}$$

---

[6] In order to avoid possible confusions between the lattice spacing and the complex number unity, only in this deduction I will use x_i as the lattice spacing.

For the term $\sum_i a_i^\dagger a_{i+1}$, it is enough to take the dagger of the equation above. Now replacing these results in the Hamiltonian, we find that:

$$H = \sum_k -[\alpha e^{ik} + \alpha e^{-ik}] b_k^\dagger b_k. \tag{3.58}$$

Using Euler's formula:

$$H = \sum_k [-2\alpha \cos(k)] b_k^\dagger b_k \qquad \to \epsilon(k) = -2\alpha \cos(k). \tag{3.59}$$

Thanks to the periodicity of the chain, $e^{ik(x_N+1)=e^{ikx_1}}$ has to be true. This equality is obtained taking:

$$k = \frac{2\pi l}{N}, \qquad l = 1, 2, 3..., N. \tag{3.60}$$

II- Open Boundary Conditions: As a guide, imagine a priori a system with 5 sites. So the task is to diagonalize

$$W = \begin{pmatrix} 0 & -\alpha & 0 & 0 & 0 \\ -\alpha & 0 & -\alpha & 0 & 0 \\ 0 & -\alpha & 0 & -\alpha & 0 \\ 0 & 0 & -\alpha & 0 & -\alpha \\ 0 & 0 & 0 & -\alpha & 0 \end{pmatrix} \tag{3.61}$$

and we need to resolve $H|\psi\rangle = \epsilon|\psi\rangle$, $|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix}$ Replacing in the eigenvalue equation:

$$\begin{pmatrix} 0 & -\alpha & 0 & 0 & 0 \\ -\alpha & 0 & -\alpha & 0 & 0 \\ 0 & -\alpha & 0 & -\alpha & 0 \\ 0 & 0 & -\alpha & 0 & -\alpha \\ 0 & 0 & 0 & -\alpha & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix} = \epsilon \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix} \tag{3.62}$$

We are able to solve this equation line by line. Except for the boundiers, we find:

$$-\left(\alpha c_{n-1} + \alpha c_{n+1}\right) = \epsilon c_n. \tag{3.63}$$

Unlike the case of periodic boundary conditions, to solve this type of equation, we can not use just a complex exponential as ansatz, because now we need $c_0 = c_{N+1} = 0$, and thus, we will use two of them. In other words, we shall use the coefficient $c_n = \tilde{A}e^{ikn} + \tilde{B}e^{-ikn}$. Then we replace this in the equation above and obtain:

$$-\alpha(e^{-ikn} + e^{-ikn})\Big(\tilde{A}e^{ikn} + \tilde{B}e^{-ikn}\Big) = \epsilon(\tilde{A}e^{ikn} + \tilde{B}e^{-ikn}). \tag{3.64}$$

Dividing both sides by $\tilde{A}e^{ikn} + \tilde{B}e^{-ikn}$, we find:

$$-\left(\alpha e^{-ik} + \alpha e^{ik}\right) = \epsilon(k). \tag{3.65}$$

To simplify this equation, we use Euler's equation and obtain:

$$\epsilon(k) = -2\alpha\cos(k) \qquad k \in [-\pi, \pi] \tag{3.66}$$

Now we wish to find c_n. For this system, the initial conditions are $c_0 = c_{n+1} = 0$. Replacing

$$c_0 = \tilde{A} + \tilde{B} = 0 \rightarrow \tilde{B} = -\tilde{A}. \tag{3.67}$$

Thereby,

$$c_n = \tilde{A}(e^{ikn} - e^{-ikn}) = 2i\tilde{A} = A\sin(nk) \rightarrow c_{N+1} = A\sin\Big(k(N+1)\Big) = 0. \tag{3.68}$$

It is useless to take the trivial solution $A = 0$, so we do $\sin\Big(k(N+1)\Big) = 0$ and this implies that

$$k = \frac{l\pi}{(N+1)} \qquad l = 1, 2, 3, ... \tag{3.69}$$

This is useful for us because it gives us a non trivial solution.

$$c_n = A\sin\left(\frac{n\pi l}{N+1}\right) \tag{3.70}$$

The coefficients c_n do not give us a normalized $|\psi\rangle$. Then, using

$$\sum_n \mid c_n \mid^2 = 1 \quad \rightarrow A = \sqrt{\frac{2}{N+1}} \tag{3.71}$$

Our results are then:

$$S_{nl} = \sqrt{\frac{2}{N+1}}\sin\left(\frac{n\pi l}{N+1}\right) \tag{3.72}$$

and

$$\epsilon(k) = -2\alpha\cos(k). \tag{3.73}$$

3.4 Grand Canonical Ensemble

An appropriate statistical method to describe one system is based on the type of the border of the system and the reservoir that it is in contact. For instance, if the border allows the system to exchange only heat with the environment, then we describe the system using the so called *canonical ensemble*. On the other hand, if one has a reservoir of heat and volume, then we use the ensemble of pressures. For the interest of this dissertation, I want to derive the well known *grand canonical ensemble*

The grand canonical ensemble is based on a heat and particle reservoir and a system with a permeable and diathermal border. So neither the internal energy nor the number of particles is fixed. The ideia is shown in Fig. 3.2.

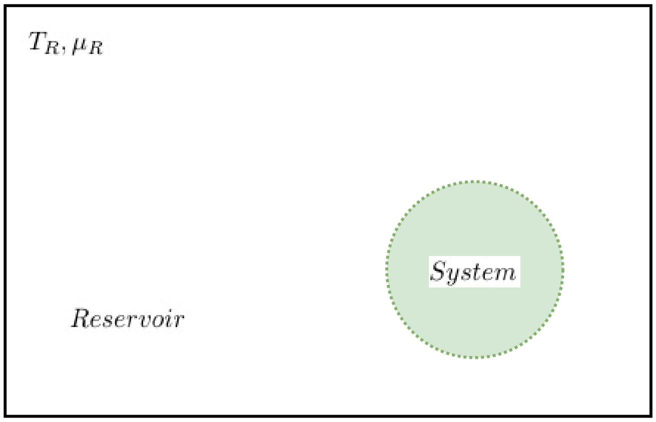

Figure 3.2: A system with a permeable and diathermal border in contact with a heat and particle reservoir.

3.4.1 Formulation of the Grand Canonical Ensemble

Consider the universe of figure 3.2 such that the total energy and number of particles obey a closure relation

$$E_S + E_R = E_0 \tag{3.74}$$

$$N_S + N_R = N_0, \tag{3.75}$$

where $E_{S,R}$ and $N_{S,R}$ are the energy and number of particles of the system and the reservoir and E_0 and N_0 are the total energy and number of particles of the system and reservoir together.

To formulate the grand canonical ensemble, we start using the fundamental postulate of statistical mechanics, the probability of the system S being found at a particular microscopic state j, with energy E_j and a number of particles N_j can be written in the shape

$$P_j = c\Omega_R(E_0 - E_j, N_0 - N_j) \tag{3.76}$$

because the probability of the system to be at j is the same that the reservoir to be with energy $E_0 - E_j$, number of particles $N_0 - N_j$ and possible microstates $\Omega_R(E_0 - E_j, N_0 - N_j)$.

Taking the logarithm of it, we find

$$\ln P_j = \mathcal{C} + \ln(\Omega(E_0 - E_j, N_0 - N_j)) \tag{3.77}$$

and since the total energy $E_0 >> E_j$ and $N_0 >> N_j$, we can expand in Taylor series.

$$\ln P_j = \mathcal{C} + \left(\frac{\partial \ln \Omega_R}{\partial E}\right)_{E_0,N_0} (-E_j) + \left(\frac{\partial \ln \Omega_R}{\partial N}\right)_{E_0,N_0} (-N_j)... \tag{3.78}$$

Using Euler's relation

$$E = -\mathcal{P}V + TS + \mu N \tag{3.79}$$

and

$$S = k_B \ln \Omega \tag{3.80}$$

we obtain

$$\frac{\partial \ln \Omega_R}{\partial E} = \frac{1}{k_B T}, \qquad \frac{\partial \ln \Omega_R}{\partial N} = \frac{-\mu}{k_B T}. \tag{3.81}$$

Replacing these in the eq. 3.78 we get

$$\ln P_j = \mathcal{C} - \frac{E_j}{k_B T} + \frac{\mu N_j}{k_B T} \tag{3.82}$$

and thus

$$P_j = Ce^{-\beta(E_j - \mu N_j)}, \tag{3.83}$$

where $\beta = k_B T$ [7].Thanks to the normalization condition

$$C = \frac{1}{\sum_j e^{-\beta(E_j - \mu N_j)}}, \tag{3.84}$$

and

$$P_j = \frac{e^{-\beta(E_j - \mu N_j)}}{\sum_j e^{-\beta(E_j - \mu N_j)}}. \tag{3.85}$$

For completeness,

$$\Xi = \sum_j e^{-\beta(E_j - \mu N_j)} \tag{3.86}$$

is called *grand partition function.*

3.4.2 Occupation Number and Internal Energy for Fermions

The grand partition function, given by the eq. 3.86 is not just a function that normalizes the distribution, it also provides information about the system such that averages of energy and particle for a system.

Opening the grand partition function in terms of the occupation of each state and the total number of particles, we find

$$\Xi = \sum_{N=0}^{\infty} \quad \sum_{n_j; \sum n_j = N} \exp[-\beta(\epsilon_1 - \mu)n_1 - \beta(\epsilon_2 - \mu)n_2 ...] \tag{3.87}$$

that is equivalent to

$$\Xi = \sum_{n_1, n_2, n_3, ...} \exp[-\beta(\epsilon_1 - \mu)n_1 - \beta(\epsilon_2 - \mu)n_2 ...] = \prod_j \Big\{ \sum_n \exp[-\beta(\epsilon_j - \mu)] \Big\}. \tag{3.88}$$

It is also possible to note that

$$\ln \Xi = \sum_j \Big(\ln \sum_n \exp[-\beta(\epsilon_j - \mu)n] \Big) \tag{3.89}$$

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[7] For the purpose of this dissertation, k_B is set to one.

and then

$$\frac{-1}{\beta}\frac{\partial \ln \Xi}{\partial \epsilon_j} = \sum_n n e^{-\beta(\epsilon_j - \mu)} = \langle n_j \rangle \,. \tag{3.90}$$

So, once one has in hands the grand partition function, just using a logarithm and a derivative, it is possible to know the average of the occupations for a state j. Of particular interest to this dissertation, for fermions the occupation can be only zero or one. Using this in the result above, the average will be

$$\langle n_j \rangle = \frac{-1}{\beta}\frac{\partial \ln(1 + e^{-\beta(\epsilon_j - \mu)})}{\partial \epsilon_j}, \tag{3.91}$$

and finally,

$$\langle n_j \rangle = \frac{1}{e^{\beta(\epsilon_j - \mu)} + 1}. \tag{3.92}$$

This result is the well known occupation for the Fermi-Dirac statistics, that directly obeys the Pauli Principle of Exclusion, because the exponential has values in the interval $]0, \infty[$, making $0 \leq \langle n_j \rangle \leq 1$.

As well as the occupation number, the internal energy is also a quantity of interest. Investigating the changes of the internal energy, it is possible to know properties such as heat capacity or fluxes of heat or even fluxes of particles.

The internal energy is just the average of the energy of the system. We can systematically obtain the internal energy having in hands the average of occupation of each level. Thus, once one knows the average of occupation of a state j and its energy, the product of both gives us the contribution of this state for the system and therefore, summing all these states, the internal energy of the system is obtained .

$$U = \sum_j \epsilon_j \langle n_j \rangle \tag{3.93}$$

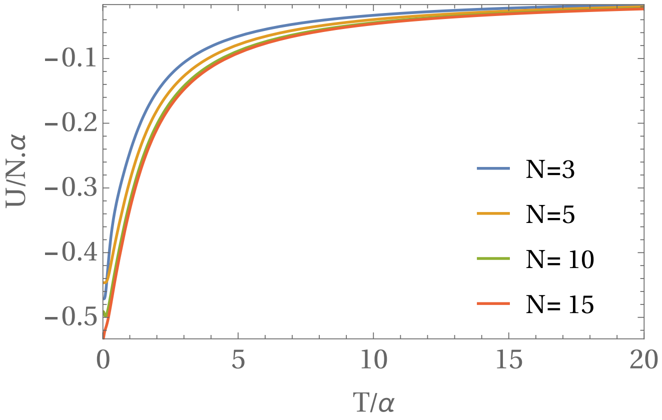

Figure 3.3: Energy per site for systems with different number N of sites and prepared at $\mu/\alpha = 1$ in function of temperature

3.4.3 Thermodynamics Limit

We previously found the possible values of ϵ_k for our tight-binding Hamiltonian and determined that k is a discrete variable, but it also depends of the number N of sites of the system. For the so called thermodynamics limit, which has $N \to \infty$, the difference between two adjacent momentums are too small because $\Delta k \propto 1/N$. Therefore, in this limit,we can treat k as a continuous variable and convert the sums into integrals as shown below.

$$\begin{aligned} k &= \frac{\pi}{N+1} m \qquad m = 1, 2, 3, \dots N \\ \Delta k &= \frac{\pi}{N+1} \to \frac{N+1}{\pi} \Delta k = 1 \end{aligned} \tag{3.94}$$

Now we multiply the internal energy by one so that we will obtain a Riemann's sum.

$$\begin{aligned} U &= \lim_{N\to\infty} \frac{N+1}{\pi} \sum_k \frac{\epsilon_k}{e^{(\epsilon_k - \mu)/T} + 1} \Delta k = \\ &= \frac{N}{\pi} \int_0^\pi \frac{\epsilon_k}{e^{(\epsilon_k - \mu)/T} + 1} dk. \end{aligned} \tag{3.95}$$

The same method is valid for the $\langle \hat{N} \rangle$. So

$$\langle \hat{N} \rangle = \frac{N}{\pi} \int_0^\pi \frac{1}{e^{(\epsilon_k - \mu)/T} + 1} dk. \tag{3.96}$$

It is already known that U and $\hat{N}$ are extensive. As it can be seen in fig. 3.3, as soon as the system gets larger, the energy per site converges and, thanks to this fact, it is interesting for us to know the energy and occupation per site. To obtain this we just divide both sides by N. Therefore,

$$\frac{U}{N} = \frac{1}{\pi}\int_0^{\pi} \frac{\epsilon_k}{e^{(\epsilon_k-\mu)/T}+1}dk, \quad \frac{\langle \hat{N}\rangle}{N} = \frac{1}{\pi}\int_0^{\pi} \frac{1}{e^{(\epsilon_k-\mu)/T}+1}dk. \tag{3.97}$$

3.4.4 Sommerfeld Expansion

It is very common in condensed matter physics the appearance of integrals that depends on the occupation given by the Fermi-Dirac statistics [53] [8]. For example, integrals like

$$I = \int_{-\infty}^{\infty} \frac{f(E)}{e^{(E-\mu)/T}+1}dE \tag{3.98}$$

are in general too difficult to compute analytically. In order to have some possible analytical results, Arnold Sommerfeld developed an expansion for low temperatures. For the purpose of having an approximation of eq. 3.98, we start making $(E-\mu)/T = x$ and separate in two integrals. We then obtain

$$I = T\int_{-\infty}^{0} \frac{f(\mu+Tx)}{e^x+1}dx + T\int_{0}^{-\infty} \frac{f(\mu+Tx)}{e^x+1}dx. \tag{3.99}$$

In the first integral we also make another substitution $x \to -x$ and get

$$I = T\int_{0}^{\infty} \frac{f(\mu-Tx)}{e^{-x}+1}dx + T\int_{0}^{\infty} \frac{f(\mu+Tx)}{e^x+1}dx. \tag{3.100}$$

Now the trick is to write $\frac{1}{e^{-x}+1} = 1 - \frac{1}{e^x+1}$. Then, we obtain

$$I = T\left[\int_0^{\infty} f(\mu-Tx)dx + \int_0^{\infty} \frac{f(\mu+Tx)-f(\mu-Tx)}{e^x+1}dx\right]. \tag{3.101}$$

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[8] In this section I make a simpler deduction of Sommerfeld Expansion. For a more detailed deduction, see [53]

For small temperatures, thanks to Taylor series, it is possible to write $f(\mu+Tx)-f(\mu-Tx) \approx 2Txf'(\mu)$. Thus ,

$$I = T\left[\int_0^\infty f(\mu - Tx)dx + 2Tf'(\mu)\int_0^\infty \frac{x}{e^x+1}dx\right]. \tag{3.102}$$

Remembering the Riemann's zeta function, the last integral will be $\pi^2/12$ and then we find

$$I = \int_{-\infty}^{\mu} f(E)dE + \frac{\pi^2 T^2}{6} f'(\mu). \tag{3.103}$$

3.4.4.1 Sommerfeld Expansion in the Internal Energy

As an application of the Sommerfeld expansion, let us consider the $1D$ chain, worked preveously with spectrum $\epsilon_k = -2\cos(k)$ which in $k \in [0,\pi]$.

The internal energy per site is given by

$$\frac{U}{N} = \int_0^\pi \frac{-2\cos(k)}{e^{(-2\cos(k)-\mu)/T}+1}dk. \tag{3.104}$$

This integral is clearly very difficult. We have then two options: i) compute it numerically ii) for small temperatures, use the Sommerfeld expansion.

The internal energy per site with Sommerfeld expansion is

$$\frac{U}{N} = \frac{1}{\pi}\left(\frac{2\pi^2T^2}{3(4-\mu^2)^{3/2}} - \sqrt{4-\mu^2}\right). \tag{3.105}$$

But, what is a low temperature? In Fig.(3.4.4.1) and Fig.(3.5) we can see a comparasion between the exact and the approximated results.

Therefore, low temperature depends on the value of the chemical potential. We can see through Eq.(3.105) that when $|\mu| \to 2$, the value of the internal energy diverges in the Sommerfeld expansion.The smaller the value of $|\mu|$is, the better the approximation will be.

As we can see in Fig.(3.4.4.1) and Fig.(3.5), the approximation also depends on the scale of energy α. For instance, if one system has α = 10meV [9], the approximation is valid for

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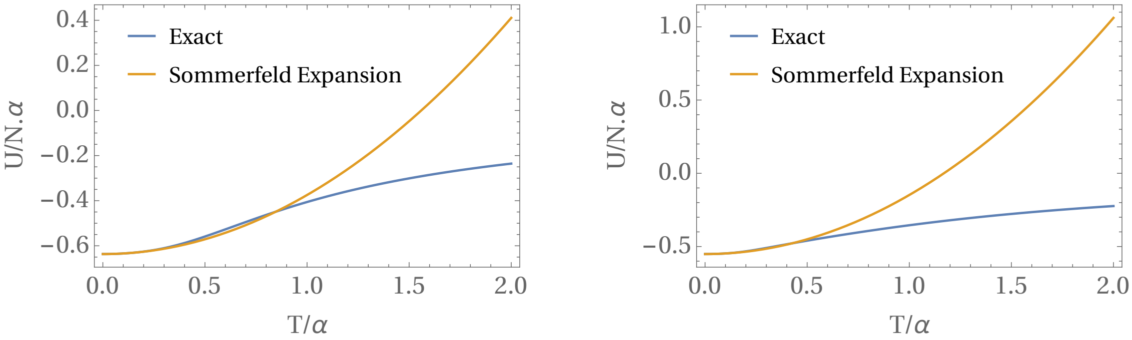
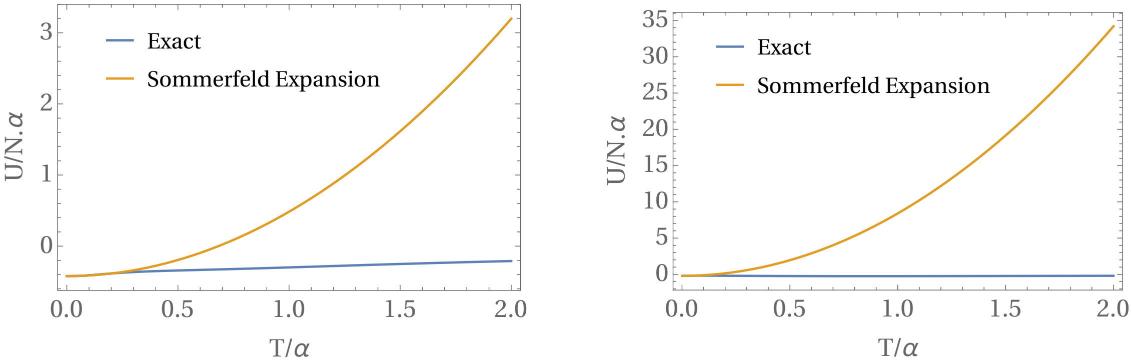
[9] $1eV = 1,6.10^{-19}J$.



(a) System prepared at $\mu = 0$.

(b) System prepared at $\mu = 1\alpha$.

Figure 3.4: Some comparisons between the exact and approximate results.



(a) System prepared at $\mu = 1.5\alpha$.

(b) System prepared at $\mu = 1.9\alpha$.

Figure 3.5: Some comparisons between the exact and approximated results.

$T = 10 - 100K$. If we go further and consider $\alpha = 1$eV (which is the order of a semiconductor band gap), this aproximation gives us good results for $T = 1000 - 10.000K$.

Chapter 4

Quantum Thermodynamics

In this chapter we will discuss some relevant topics in quantum thermodynamics, starting with a brief discussion of classical concepts, such as Onsager's theorem and then moving on to a discussion of fluctuations theorems.

4.1 Onsager's Theorem

Equilibrium thermodynamics provides us with broad range of tools that allow us to describe and predict properties of equilibrium systems or for slowly driven processes. However, as argued in the introduction, sometimes it is much more interesting to study out of equilibrium processes than the equilibrium one, as well as what type of phenomena generate the processes that drive the system until the equilibrium.

4.1.1 Affinities and fluxes

Before we show the emergence of Onsager's theorem, let us discuss some quantities that describe irreversible processes. Basically, two kinds of parameters are required: a generalized force, which drives the processes and the currents developed in the system in response to this force [3] [1].

Consider a composite system composed of 2 subsystems. Let X_k and X'_k denote a set of extensive parameters of systems 1 and 2, such as e.g. the internal energy. If we assume

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[1] This section was based in [3] and some notes of Professor Gabriel Teixeira Landi.

that the composite system is isolated, then these extensive quantities must satisfy the closure relation:

$$X_k + X'_k = X^0_k. \tag{4.1}$$

The equilibrium values of X_k and X'_k are determined by the principle of maximum entropy, which requires the vanishing of the following quantity:

$$\mathcal{F}_k \equiv \left(\frac{\partial S^0}{\partial X_k}\right)_{X^0_k} = \left(\frac{\partial (S+S')}{\partial X_k}\right)_{X^0_k} = \frac{\partial S}{\partial X_k} - \frac{\partial S'}{\partial X_{k'}} = F_k - F_{k'}, \tag{4.2}$$

where S and S' are the entropy of each system and S^0 is the total entropy Thus, if $\mathcal{F}_k$ is zero,then the systems are in equilibrium, but if $\mathcal{F}_k$ is different from zero, then an irrersible process occurs, taking the system toward the equilibrium state. The quantity $\mathcal{F}_k$ acts like a generalized force that drives the processes and receive the name *affinity.*

For example, consider two systems separated by a diathermal wall, and let X_k be the internal energy U. Then, since $\partial S/\partial U = 1/T$, the affinity will be:

$$\mathcal{F} = \frac{1}{T} - \frac{1}{T'}, \tag{4.3}$$

and therefore, the systems are in equilibrium if $T = T'$, which is what we expect from our intuition. Similarly, if X_k is the number of particles, then the associated affinity is $\left[\frac{\mu_{k'}}{T'} - \frac{\mu_k}{T}\right]$, where μ is the chemical potential.

The other central quantity in this framework is the response of the system to the affinities, which is characterized by the fluxes of the extensive quantities X_k:

$$J_k \equiv \frac{dX_k}{dt}. \tag{4.4}$$

The identification of the affiniies in a particular system is frequently rendered more convenient by considering the rate of entropy production. Taking the derivative of $S_0(X_0, X_1, X_2, ...)$ with respect to t, we obtain

$$\frac{dS_0}{dt} = \sum_k \frac{\partial S}{\partial X_k}\frac{dX_k}{dt} \tag{4.5}$$

and consequently

$$\frac{dS_0}{dt} = \sum_k \mathcal{F}_k J_k. \tag{4.6}$$

4.1.2 Markovian Systems

For certain systems, the fluxes at a given instant of time depend only on the values of the affinities at that instant, so the affinities as well will also depend only on the time of interest.

Here it should be noted that we do not assume that each flux depends only on its own affinity but rather that depends on all affinities.

$$J_k = J_k(\mathcal{F}_0, \mathcal{F}_1, ...; F_0, F_1, ...) \tag{4.7}$$

If the affinities vanish, the fluxes J_k vanish as well. Thus, for sufficiently small affinities we may expand the currents in a Taylor series as

$$J_k = \sum_j L_{j,k}\mathcal{F}_j + \frac{1}{2!}\sum_{i,j} L_{i,j,k}\mathcal{F}_i\mathcal{F}_j + ..., \tag{4.8}$$

where

$$L_{j,k} = \left(\frac{\partial J_k}{\partial \mathcal{F}_j}\right)_0, \qquad L_{i,j,k} = \left(\frac{\partial^2 J_k}{\partial \mathcal{F}_i \partial \mathcal{F}_j}\right)_0 \tag{4.9}$$

and the coefficients $L_{j,k}$ are called *kinect coefficient* and $L_{i,j,k}$ are called *second order kinect coefficient*. To first order, we retain only the linear terms and assume that the current is given by

$$J_k = \sum_j L_{j,k}\mathcal{F}_j. \tag{4.10}$$

The most important result of Onsager [54, 55] known as Onsager's reciprocity theorem, is that

$$L_{i,j} = L_{j,i}, \tag{4.11}$$

which is physically unintuitive and, quite remarkably, is a direct consequence of the invariance of the laws of physics under time reversal.

For the interest of this dissertation, I will discuss the Onsager Coefficients and fluxes for exchange of particles and energy. First of all, we remember again from the thermodynamics that

$$dS = \frac{dU}{T} - \frac{\mu}{T}dN. \tag{4.12}$$

From the definition of a differential we get

$$\frac{\partial S}{\partial U} = \frac{1}{T}, \qquad \rightarrow \qquad \frac{\partial S}{\partial N} = -\frac{\mu}{T} \tag{4.13}$$

and consequently, the affinities are

$$\mathcal{F}_1 = -\frac{\mu_A}{T_A} + \frac{\mu_B}{T_B}, \quad \rightarrow \quad \mathcal{F}_2 = \frac{1}{T_B} - \frac{1}{T_A}. \tag{4.14}$$

Using the equation Eq.(4.10), we have

$$\begin{aligned} J_N &= L_{11}F_1 + L_{12}F_2 \\ J_U &= L_{21}F_1 + L_{22}F_2, \end{aligned} \tag{4.15}$$

where $L_{12} = L_{21}$. Considering a small difference of temperatures and chemical potential, let us write the temperatures T_A and T_B as $T_A = T + \frac{\delta T}{2}$ and $T_B = T - \frac{\delta T}{2}$ and the chemical potentials μ_A and μ_B as $\mu_A = \mu + \frac{\delta\mu}{2}$ and $\mu_B = \mu - \frac{\delta\mu}{2}$. We then find

$$\mathcal{F}_1 = \frac{\delta\mu}{T} - \frac{\mu}{T^2}\delta T, \qquad \mathcal{F}_2 = \frac{\delta T}{T^2}. \tag{4.16}$$

Substituting in Eq.(4.15) leads to

$$\begin{aligned} J_N &= L_{11}\frac{\delta\mu}{T} + (L_{12} - \mu L_{11})\frac{\delta T}{T^2} \\ J_U &= L_{21}\frac{\delta\mu}{T} + (L_{22} - \mu L_{21})\frac{\delta T}{T^2}. \end{aligned} \tag{4.17}$$

In this framework it is important to distinguish between flow of energy and flow of heat. Energy can be exchanged through the particles transport and through thermal vibrations. In this dissertation we will analyze the fluxes of heat and particles. To obtain these fluxes correctly, we can use the first law of thermodynamics and obtain $J_U = J_Q + \mu J_N$. Replacing it in the fluxes, we get:

$$\begin{aligned} J_N &= L_{11}\frac{\delta\mu}{T} + (L_{12} - \mu L_{11})\frac{\delta T}{T^2} \\ J_Q &= (L_{21} - \mu L_{11})\frac{\delta\mu}{T} + (L_{22} + \mu^2 L_{11} + \mu L_{11})\frac{\delta T}{T^2} \end{aligned} \tag{4.18}$$

and we can rewrite it as

$$\begin{aligned} J_N &= L'_{11}\frac{\delta\mu}{T} + L'_{12}\frac{\delta T}{T^2} \\ J_Q &= L'_{21}\frac{\delta\mu}{T} + L'_{22}\frac{\delta T}{T^2}. \end{aligned} \tag{4.19}$$

and so we can see that $L'_{21} = L'_{12}$ and, therefore, the Onsager's theorem is also valid for this change of variables.

4.2 Fluctuations theorems

Except in the vinicity of phase transitions, the fluctuations in thermodynamic quantities usually scale with the number of particles proportionally to $1/\sqrt{N}$. For macroscopic systems, these fluctuations are therefore irrelevant, which is why they can usually be neglected in experiments which deal with macroscopic systems. Once the system has few particles, the fluctuations over the measurements become comparable with the quantity measured and a probabilistic approach is needed. There is a class of relations that tell us about the rates of probabilities between a process and its reversal. These relations are called *fluctuations theorems* and can be roughly summarized by [6] :

$$\frac{P_F(\Sigma)}{P_B(-\Sigma)} = e^{\Sigma} \tag{4.20}$$

where $P_F(\Sigma)$ is the entropy produced in a certain "forward" process and $P_B(-\Sigma)$ is the entropy produced in the corresponding time-reversed process.

One of the most, if not the most, known fluctuation theorem is the one of authorship of

Crooks [7] concerning the distribution of work done in a system. It reads:

$$\frac{P_F(W)}{P_B(-W)} = e^{-\beta(W-\Delta F)} \tag{4.21}$$

where β is the inverse of the temperature, ΔF is the variation of the free energy between the initial and final states, $P(W)$ is the probability of a work to be done and $P(-W)$ the probability of the reversal process. The Crooks fluctuation theorem also implies

$$\langle e^{-\beta(W-\Delta F)} \rangle = 1, \tag{4.22}$$

which is known as *Jarzynski Equality.* Historically, the Jarzynski equality came before the fluctuation theorem derived by Crooks [8]. Even so, Crooks showed that, considering a Markovian dynamics and microscopic reversibility , we may obtain Eq.(4.21) and consequently Eq.(4.22).

Fluctuations theorems have been studied and verified experimentally in the last two decades and were explored in variables like work, heat, flux of matter and , recently, also for initially correlated systems [56].

4.2.1 Jarzynski's Classical and Quantum Fluctuation Theorems for Heat Exchange

In this section I will derive the fluctuation theorem for heat exchange, using the classical and quantum approach, as done by Jarzynski [6]. This section is also a preparatory for the next one, where I will consider an exchange of energy and particles.

Classical Protocol: Consider two finite bodies A and B prepared in equilibrium with thermal reservoirs with temperatures T_A and T_B ($T_A > T_B$). At an initial time $t = 0$, the systems are placed in thermal contact during an interval τ, and then, they are disconnected. Let Q denote the net heat transferred from A to B and consider that this protocol is repeated many times. Then, let $p_\tau(Q)$ be the observed distribution over the ensemble of repetitions.

In order to derive an equation with the shape of Eq.(4.20), let us consider that the microstate of the system A is specified in the phase space by z_A, which contains the positions and momenta of all degrees of freedom of this system and $H_A(z_A)$ is the Hamiltonian of this system, whose value defines the energy of A in such microstate. We also define z_B and $H_B(z_B)$ in the same manner for the system B. Finally, let $h_{int}(z_A, z_B)$ be a small interaction that describes the thermal contact present in the interval considered at the protocol.

Let $y(z_A, z_B)$ specify a point in the full phase space and $y_f(t)$ the evolution of the microstate of the full system, described by a full Hamiltonian $H(y) = H_A(z_A) + H_B(z_B) + h_{int}(y)$, from $t = 0 \to t = \tau$. As made by Crooks, we will consider a time-reversal invariance. This assumption has a crucial consequence which is that *for any trajectory $y(t)$ which is a solution of Hamilton's equation there is a time-reversed $y_b(t)$ that is also a solution.*[2] A time-reversal operation will be denoted by a (*) and its action for positions and momenta are $(q, p)^* = (q, -p)$. For this derivation, we will consider that the Hamiltonians are time-reversal invariant. Moreover, $y_b(t) = y^*(\tau - t)$ and, as a straight consequence, we have $y_b(0) = y_f(\tau)^*$ and $y_b(\tau) = y_f(0)^*$.

As mentioned above, the considered initial thermal states for A and B. Using the thermal distribution given by Gibbs, the initial probability $P(y(0))$ of obtaining an initial state $y(0)$ is given by:

$$P(y(0)) = \frac{1}{Z_A Z_B} e^{-E_A(z_A(0))/T_A} e^{-E_B(z_B(0))/T_B}, \tag{4.23}$$

where $Z_{A,B}$ are the partition function for each system. The ratio of probabilities between the initial conditions is given by:

$$\frac{P(y_f(0))}{P(y_b(0))} = e^{\Delta E_B/T_B} e^{\Delta E_A/T_A} \tag{4.24}$$

where $\Delta E_A = E_A(z_A(\tau)) - E_A(z_A(0))$ with similar definition for the system B. With the assumption of a small interaction between the two systems (weak coupling), we can approximate the change of energy of A and B by $\Delta E_B = -\Delta E_A \equiv Q$. Then, we can rewrite

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[2] In this section I am using the subindices f and b with the meaning of *foward* and *backward* as reference of the evolution of the process.

Eq.(4.24) as

$$\frac{P(y_f(0))}{P(y_b(0))} = e^{\Delta\beta Q(y_f(0))}, \tag{4.25}$$

where $Q(y)$ denotes the value of Q during the process with its initial condition. Moreover, we have $Q(y_f(0)) = -Q(y_b(0))$ and

$$p_\tau(Q) = \int dy_f(0)P(y_f(0))\delta[Q - Q(y_f(0))] = e^{\Delta\beta Q}\int dy_b(0)P(y_b(0))\delta[Q + Q(y_b(0))], \tag{4.26}$$

which implies [3]

$$\frac{p_\tau(Q)}{p_\tau(-Q)} = e^{\Delta\beta Q}, \tag{4.27}$$

in which $p_\tau(Q)$ means the probability of obtaining a heat Q by summing all the possibilities and the same is considered for the time-reversal case.

Quantum Protocol: We consider again two finite bodies A and B prepared in equilibrium with thermal reservoirs with temperatures T_A and T_B ($T_A > T_B$). Then we measure the energy of each system and after this, we connect the two systems weakly and let them evolve during an interval τ. After this interval, we disconnect the systems and measure the energy of each system again. The heat Q transferred between A and B can be interpreted in terms of the changes of the energies of the systems.

In order to prove the quantum version, we proceed with the first part of the protocol. Since each system is prepared in equilibrium with temperatures T_A and T_B, then they can be described by density matrices $\rho_{A,B} = e^{-\beta H_{A,B}}/Z_{A,B}$. We then disconnect each system from its reservoir and measure its energy. As a result of the measurement, the systems A and B are projected onto a pure state $|n_{A,B}\rangle$. Once the systems are initially uncorrelated, the initial state of the total system is given by $|n_A n_B\rangle$. Last, we will consider that the total Hamiltonian is given by:

$$H = H_A + H_B + h_{int}, \tag{4.28}$$

where h_{int} corresponds to the interaction between the two chains and H is the full Hamiltonian.

As we did in the classical case, let us consider a time-reversal invariant Hamiltonian. Such

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[3] This result was possible due to the change of variables $dy(\tau) = dy(\tau)^* = dy(0)$

consideration can be expressed as

$$\Theta H = H\Theta \tag{4.29}$$

where H is the Hamiltonian and Θ is the time-reversal operator.

The time-reversal operator is an anti-linear operator that reverses the angular and linear momenta, while it keeps the position unaltered. An example of how this operator works is shown below:

$$\Theta(c_1 \left|\psi\right\rangle + c_2 \left|\phi\right\rangle) = c_1^*\Theta \left|\psi\right\rangle + c_2^*\Theta \left|\phi\right\rangle, \tag{4.30}$$

where $c_{1,2}$ are complex numbers and $c_{1,2}^*$ their complex conjugate. Thanks to its antiunitarity, expressions like $\left\langle\psi\right| \Theta \left|\phi\right\rangle$ are ambiguous until we specify if it acts on the right or on the left and therefore, in this proof I will use the standart product in the Hilbert space $(\left|\psi\right\rangle, \left|\phi\right\rangle)$ rather $\langle\psi|\phi\rangle$. It is also needed to comment that Θ preserves the normalization and thus

$$(\Theta \left|\psi\right\rangle, \Theta \left|\phi\right\rangle) = (\left|\psi\right\rangle, \left|\phi\right\rangle). \tag{4.31}$$

At the time $t = 0$ we join A and B and let them evolve until $t = \tau$. The total system evolves under Schrödinger's equation from the initial state $\left|n\right\rangle \equiv \left|n_A n_B\right\rangle$ until a state $\left|\Psi\right\rangle$. In $t = \tau$ we disconnect A and B and measure the energy of each system. The state $\left|\Psi\right\rangle$ is projected onto $\left|m\right\rangle \equiv \left|m_A m_B\right\rangle$.

Let us denote $P_\tau(\left|n\right\rangle \to \left|m\right\rangle)$ the probability of obtaining the transformation $\left|n\right\rangle \to \left|m\right\rangle$. So

$$P_\tau(\left|n\right\rangle \to \left|m\right\rangle) = |(\left|m\right\rangle, U_\tau \left|n\right\rangle)|^2 \frac{e^{-\beta_A E_{n,A} - \beta_B E_{n,B}}}{Z_A Z_B}, \tag{4.32}$$

where $U_\tau = e^{-iH\tau}$ (with $\hbar = 1$). Now, looking to the reversed process, the probability of obtaining $\Theta \left|m\right\rangle \to \Theta \left|n\right\rangle$ is given by

$$P_\tau(\Theta \left|m\right\rangle \to \Theta \left|n\right\rangle) = |(\Theta \left|n\right\rangle, U_\tau \Theta \left|m\right\rangle)|^2 \frac{e^{-\beta_A E_{m,A} - \beta_B E_{m,B}}}{Z_A Z_B}. \tag{4.33}$$

If we expand U_τ in Taylor series, we may observe that $U_\tau \Theta = \Theta U_{-\tau}$ and moreover

$$\begin{aligned}(\Theta\left|n\right\rangle, U_\tau\Theta\left|m\right\rangle) &= (\Theta\left|n\right\rangle, \Theta U_{-\tau}\left|m\right\rangle) \\ &= (U_{-\tau}\left|m\right\rangle, \left|n\right\rangle = (\left|m\right\rangle, U_\tau\left|n\right\rangle). \end{aligned} \tag{4.34}$$

Therefore,

$$\frac{P_\tau(\left|n\right\rangle \to \left|m\right\rangle)}{P_\tau\Theta\left|m\right\rangle \to \Theta\left|n\right\rangle} = e^{-\beta_A(E_{n,A}-E_{m,A})}e^{-\beta_B(E_{n,B}-E_{m,B})}. \tag{4.35}$$

Using the weak coupling assumption, we can define, in the same way done in the classical proof, $Q_{n\to m} \equiv -\Delta E_A = \Delta E_B = E_{m,B} - E_{n,B}$ and thus:

$$\frac{P_\tau(\left|n\right\rangle \to \left|m\right\rangle)}{P_\tau\Theta\left|m\right\rangle \to \Theta\left|n\right\rangle} = e^{Q_{n\to m}\Delta\beta}. \tag{4.36}$$

Each eigenstate has a time-reversed correspondent, so the probability of obtaining a trasfered heat Q in a protocol time τ is:

$$\begin{aligned} p_\tau(Q) &= \sum_{n,m} P_\tau(\left|n\right\rangle \to \left|m\right\rangle)\delta(Q - Q_{n\to m}) \\ &= e^{Q\Delta\beta}\sum_{\Theta n,\Theta m} P_\tau(\Theta\left|m\right\rangle \to \Theta\left|n\right\rangle)\delta(Q + Q_{\Theta m\to\Theta n}) \\ &= e^{Q\Delta\beta}p_\tau(-Q). \end{aligned} \tag{4.37}$$

Finally,

$$\frac{p_\tau(Q)}{p_\tau(-Q)} = e^{Q\Delta\beta}. \tag{4.38}$$

4.2.2 Fluctuation Theorems for Heat and Particle Exchanges for Bipartite Systems

In this dissertation we will focus on the fluctuations of heat and particle exchanged between two bodies placed in contact with each other, as done in [57]. As we will show, the heat also satisfies a fluctuation theorem, as first shown by Jarzynski and Wójcek in [6]. So, in a initial time, $t = 0$, the two systems are disconnected from the respective reservoirs and are joined and left to evolve.

Consider a bipartite system, in which one side is called A and the other is called B, have Hamiltonians H_A and H_B and the interaction between the two parts is given by a potential V. So the total Hamiltonian is given by $H = H_A + H_B + V$.

The initial total density matrix is given by

$$\rho(0) = \rho_A^{eq}(\beta_A, \mu_A) \otimes \rho_B^{eq}(\beta_B, \mu_B), \tag{4.39}$$

where

$$\rho_X^{eq}(\beta_X, \mu_X) = \frac{e^{-\beta_X H_X - \mu_X N_X}}{\Xi_X}, \quad X = A, B \tag{4.40}$$

and the Ξ_X is the grand canonical partition function of the system X. The index i_X will be used to distinguish the different eigenstates of H_X with the same energy E_X. We define then $i = (i_A, i_B)$ and $\alpha = (E_A, n_A, E_B, n_B)$.

The probability of measuring the system initially in (i, α) and evolving to (i', α') is given by

$$P_F[i', \alpha'; i, \alpha] = | \langle i', \alpha' | \, U_t \, | i, \alpha \rangle |^2 \langle \alpha | \, \rho_0 \, | \alpha \rangle . \tag{4.41}$$

On the other hand, the time reversed evolution occurs with probability

$$P_R[i, \alpha; i', \alpha'] = | \langle i', \alpha' | \, U_t \, | i, \alpha \rangle |^2 \langle \alpha' | \, \rho_0 \, | \alpha' \rangle . \tag{4.42}$$

Then the ratio is given by

$$\frac{P_F[i', \alpha'; i, \alpha]}{P_R[i, \alpha; i', \alpha']} = e^{-\beta_A \Big((E_A - E_{A'}) - \mu_A (N_A - N_{A'}) \Big)} e^{-\beta_B \Big((E_B - E_{B'}) - \mu_B (N_B - N_{B'}) \Big)} \tag{4.43}$$

We can divide the types of interaction between two systems in two ways. If the energy of interaction is large compared to the total energy, or the energy of each system, we say that we have a *strong coupling.* If the energy of interaction is small compared to the energy of the systems, we say that we have a *weak coupling.*

Using the assumption of weak coupling, we can say that

$$E_A - E_{A'} \approx -\Big(E_B - E_{B'} \Big), \tag{4.44}$$

and moreover

$$N_A - N_{A'} = -\Big(N_B - N_{B'}\Big). \tag{4.45}$$

We also define:

$$\begin{aligned} A_h &= -\beta_A + \beta_B &(4.46)\\ A_m &= \beta_A\mu_A - \beta_B\mu_B. &(4.47)\end{aligned}$$

Using these definitions and summing all cases with this exchange of energy and particles, we finally obtain

$$\frac{p[\Delta E_A, \Delta N_A]}{p[-\Delta E_A, -\Delta N_A]} = e^{-(A_h\Delta E_A + A_m\Delta n_A)}. \tag{4.48}$$

A nonequilibrium equality is obtained integrating both sides of

$$p[\Delta E_A, \Delta N_A] = p[-\Delta E_A, -\Delta N_A]e^{-(A_h\Delta E_A + A_m\Delta N_A)} \tag{4.49}$$

and we find

$$\langle e^{-(A_h\Delta E_A + A_m\Delta N_A)}\rangle = 1. \tag{4.50}$$

If we take $\mu_A = \mu_B$, we recover the previously discussed Jarzynki and Wójcik fluctuation theorem:

$$\frac{P(Q)}{P(-Q)} = e^{Q\Delta\beta}, \tag{4.51}$$

where $\Delta\beta = \beta_B - \beta_A$ and $\beta_B > \beta_A$.

Chapter 5

Open Quantum Systems

So far the discussions have been restricted to unitary dynamics, in other words, the systems interacted totally isolated and, therefore, the system is fully determined by Schrödinger's equation. Consequently, the evolution of the density matrix is given by von-Neumann's equation.

For the non-unitary dynamics, this equation is no longer valid. In this dissertation I will pay attention to the cases where the system evolves under a markovian process, which obey the semigroup property $V(t_1 + t_2) = V(t_1)V(t_2)$.

5.1 Derivation of the Lindblad Equation

The objective here is to find the most general master equation that obeys the semigroup property. Mathematically, we obtain the time evolved matrix of the system ρ_s through the application of a dynamical map, such that [1] [58]

$$\rho_s(t) = V(t)\rho_s(0) \equiv tr_B\Bigg\{U(t,0)[\rho_s(0) \otimes \rho_B]U^\dagger(t,0)\Bigg\}, \tag{5.1}$$

where $V(t)$ is the dynamical map, which gives us the evolution of the reduced density matrix and $U(t, t_0)$ is the time-evolution operator, obtained by solving Schrödinger's equation for the composite system. Given the density operator of the bath in the spectral decomposition,

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[1] This derivation as well as an alternative one can be seen in *The theory of open quantum systems*.

$\rho_B = \sum_\alpha \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$ we get:

$$\begin{aligned}\rho_s(t) &= V(t)\rho_s(0) \equiv tr_B \left\{ U(t,0)\rho_s(0) \otimes \Big(\sum_\alpha \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha| \Big) U^\dagger(t,0) \right\} &(5.2)\\ &= \sum_{\alpha,\beta} W_{\alpha,\beta}(t)\rho_s W^\dagger_{\alpha,\beta}(t), &(5.3)\end{aligned}$$

where $W_{\alpha,\beta}(t) = \sqrt{\lambda_B}\langle\phi_\alpha| U(t,0) |\phi_\alpha\rangle$ are the kraus operators, whose properties are discussed in appendix A. If the characteristic time scales over which the reservoir correlation functions decay are much smaller than the characteristic time scale of the systematic evolution, it is justified to neglect memory effects in the reduced system dynamics. If the evolution obeys the semigroup property, the map of the evolution is given by

$$V(t) = e^{\mathcal{L}t} \tag{5.4}$$

where $\mathcal{L}$ is the generator of the semigroup. The map above generates the differential equation

$$\frac{d\rho_s}{dt} = \mathcal{L}\rho_s(t), \tag{5.5}$$

that is called *Markovian quantum master equation*. In order to derive another form of the master equation, we move the problem to Liouville space. So, given a Hilbert space of dimension N, the Liouville space will have dimension N^2.

Let F_i, $i = 1, 2, ...N^2$ be a complete basis of the Liouville space. The inner product is defined as:

$$(F_i, F_j) \equiv tr_s\{F_i^\dagger F_j\} = \delta_{ij}. \tag{5.6}$$

For convenience $F_{N^2} = \frac{1}{\sqrt{N}} I_s$ and the other $tr_s F_i = 0$. Inserting a completeness in $W_{\alpha,\beta}(t) = \sqrt{\lambda_B}\langle\phi_\alpha| U(t,0) |\phi_\alpha\rangle$ we obtain:

$$W_{\alpha,\beta}(t) = \sum_{i=1}^{N^2} F_i(F_i, W_{\alpha,\beta}) \tag{5.7}$$

and therefore

$$\begin{aligned}\frac{d\rho_s}{dt} &= V(t)\rho_s = \sum_{i,j=1}^{N^2}\sum_{\alpha,\beta} F_i(F_i, W_{\alpha,\beta})\rho_s F_j^\dagger (F_, W_{\alpha,\beta})^* && (5.8)\\ &= \sum_{i,j=1}^{N^2} c_{ij} F_i \rho_s F_j^\dagger, && (5.9)\end{aligned}$$

with $c_{ij} = (F_i, W_{\alpha,\beta})(F_j, W_{\alpha,\beta})^*$. Remembering that $\frac{d\rho_s}{dt} = \mathcal{L}\rho_s(t)$ and using the deffinition of derivatives, it is shown, that

$$\begin{aligned}\mathcal{L}\rho_s &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\{V(\epsilon)\rho_s - \rho_s\}\\ &= \lim_{\epsilon\to 0}\left\{\frac{1}{N}\frac{c_{N^2,N^2} - N}{\epsilon}\rho_s + \frac{1}{\sqrt{N}}\sum_{i=1}^{N^2-1}\frac{c_{i,N^2}(\epsilon)}{\epsilon}F_i\rho_s + \frac{c_{N^2,i}(\epsilon)}{\epsilon}F_i^\dagger \rho_s\right.\\ &\qquad \left. + \sum_{i,j=1}^{N^2-1}\frac{c_{i,j}(\epsilon)}{\epsilon}F_i\rho_s F_j^\dagger\right\}. && (5.10)\end{aligned}$$

Defining the coefficients a_{ij} as

$$\begin{aligned}a_{N^2,N^2} &= \lim_{\epsilon\to 0}\frac{c_{N^2,N^2}(\epsilon) - N}{\epsilon} && (5.11)\\ a_{i,N^2} &= \lim_{\epsilon\to 0}\frac{c_{i,N^2}(\epsilon)}{\epsilon} \quad , i = 1, 2, ..., N && (5.12)\\ a_{i,j} &= \lim_{\epsilon\to 0}\frac{c_{i,j}(\epsilon)}{\epsilon} \quad , i, j = 1, 2, ..., N && (5.13)\end{aligned}$$

and defining the quantities $F = \frac{1}{\sqrt{N}}\sum a_{i,N^2}F_i$ and $G = \frac{1}{2N}a_{N^2,N^2}I_s + \frac{1}{2}(F^\dagger + F)$, as well as the Hermitian operator $H = \frac{1}{2i}(F^\dagger - F)$, one finds:

$$\mathcal{L}\rho_s = -i[H, \rho_s] + \{G, \rho_s\} + \sum_{i,j=1}^{N^2-1} a_{ij}F_i\rho_s F_j^\dagger. \tag{5.14}$$

Since the semigroup is trace preserving:

$$tr_s\{\mathcal{L}\rho_s\} = tr\left\{\left(2G + \sum_{i,j=1}^{N^2-1} a_{ij}F_i\rho_s F_j^\dagger\right)\rho_s\right\} = 0. \tag{5.15}$$

Hence, we get the first standard form:

$$\mathcal{L}\rho_s = -i[H,\rho_s] + \sum_{i,j=1}^{N^2-1} a_{ij}\Big(F_i\rho_s F_j^{\dagger} - \frac{1}{2}\{F_j^{\dagger}F_i,\rho_s\}\Big). \tag{5.16}$$

Since the matrix $a = (a_{ij})$ is positive, then it can be diagonalized by a unitary transformation $uau^{\dagger}$. This implies that $F_i = \sum_k^{N^2-1} u_{ki}L_k$ and the equation above is written as

$$\frac{d\rho_s}{dt} = -i[H,\rho_s] + \sum_{k}^{N^2-1} \gamma_k\left(L_k\rho_s L_k^{\dagger} - \frac{1}{2}\{L_k^{\dagger}L_k,\rho_s\}\right). \tag{5.17}$$

The equation (5.17) is the one called quantum master equation in the Lindblad form. The first term on the right hand is the responsible for the unitary evolution and it is the same obtained in the von-Neumann equation. The second one, sometimes written as $D(\rho_s)$ for short, is the responsible for the coupling with the environment. Moreover, γ_k is a constant which measures the coupling strength with the bath. When $\gamma_k \to 0$, then the system is uncoupled with the bath and we recover the unitary dynamics and the von Neumann equation, as it could be expected.

There are some properties that the $D(\rho_s)$ must obey. One of those is that it must be hermitian, because ρ_s is hermitian. Furthermore,

$$\mathrm{tr}\{D(\rho_s)\} = 0 \tag{5.18}$$

because it will ensure that

$$\frac{d}{dt}tr(\rho) = 0 \to tr(\rho_s) = cte \tag{5.19}$$

and consequently, the $D(\rho_s)$ is a trace preserving map.

5.1.1 Mean values at non-unitary dynamics

One of the first things we learn in statistical mechanics is how to take averages of operators. It is simply [59]

$$\langle \mathcal{O}\rangle = tr\{\mathcal{O}\rho\}, \tag{5.20}$$

where $\mathcal{O}$ is a generic operator. It is also possible to obtain the time-evolution of the average of operators in non-unitary dynamics.

$$\frac{d}{dt}\langle\mathcal{O}\rangle = \frac{d}{dt}tr[\mathcal{O}\rho(t)] = tr\Big[\mathcal{O}\frac{d\rho}{dt}\Big] \tag{5.21}$$

Using then the Lindblad equation, we get:

$$\mathrm{tr}\Big[\mathcal{O}\frac{d\rho}{dt}\Big] = i\mathrm{tr}\Big\{\mathcal{O}[H,\rho]\Big\} + \mathrm{tr}\Big\{\mathcal{O}D(\rho)\Big\}. \tag{5.22}$$

Let us start identifying more clearly the first term of the right side of the equation.

$$-i\mathrm{tr}\Bigg\{\mathcal{O}[H,\rho]\Bigg\} = i\mathrm{tr}\Bigg\{[H,\mathcal{O}]\rho\Bigg\} = i\langle[H,\mathcal{O}]\rangle \tag{5.23}$$

So the unitary part of the evolution of the system is only the average of the commutator of the Hamiltonian with the operator, which is nothing but Heisenberg's equation for closed systems. The non-unitary part will be:

$$\mathrm{tr}\Bigg\{\mathcal{O}D(\rho)\Bigg\} = \mathrm{tr}\Bigg\{\mathcal{O}\Big[L\rho L^\dagger - \frac{1}{2}(L^\dagger L\rho + \rho L^\dagger L)\Big]\Bigg\}. \tag{5.24}$$

Using the cyclic property of the trace, one finds that:

$$\mathrm{tr}\Bigg\{\mathcal{O}D(\rho)\Bigg\} = \langle L^\dagger\mathcal{O}L - \frac{1}{2}(L^\dagger L\mathcal{O} + \mathcal{O}L^\dagger L)\rangle. \tag{5.25}$$

Let us call the operator between the brackets as *adjoint dissipator*, defined as:

$$\tilde{D}(\mathcal{O}) = L^\dagger\mathcal{O}L - \frac{1}{2}(L^\dagger L\mathcal{O} + \mathcal{O}L^\dagger L), \tag{5.26}$$

and then, the time-evolution of a generic operator $\mathcal{O}$ is

$$\frac{d}{dt}\langle\mathcal{O}\rangle = i\langle[H,\mathcal{O}]\rangle + \gamma\langle\tilde{D}(\mathcal{O})\rangle. \tag{5.27}$$

5.2 Decoherence and Dephasing Noise

For most physical experiments, scientists have been searching for the conditions that minimize the interference of the external environment. For example, to study a uniform movement we need to search a place without wind and a surface with the least possible friction. To study free fall it is interesting to have a body which will be less affeted by the air resistance than the others. We can also imagine insulating materials for the study of thermodynamics and so on. The study of classical systems gave us an intuition of isolated systems, which basically gives us the possibility to study only the phenomena of interest.

In the twentieth century, with the development of quantum mechanics, some difficult questions emerged in the scientific medium. Maybe, one of the most important is the peculiar difficulty to find quantum properties, such as the superposition in macroscopic systems. The so-called quantum-to-classical transition is a very difficult question and Schrödinger's cat is a well known example of this.

Schrödinger imagined a cat confined in a box. Inside the box, the decay of an unstable atom serves like a trigger for a hammer that will break a vial of poison, and once the poison is released, the cat will be dead. By the rules of quantum mechanics, the atom will be in a superposition of "decayed" and "not decayed". The quantum entanglement implies that superposition spreads to the total system containing the cat, the hammer and the poison.

In this *gedanken experiment*, an external observer is the responsible for opening the box and measure the state and ensure that it is "classical", in other words, which the cat will be alive *or* dead.

In Schrödinger's cat, the observer has only the role to make a projective measurement and has nothing to do with the "openess" of the system, that is responsable to quantum-to-classical transition.

Through decades, it has been slowly realized that the isolated system assumption is a crucial obstacle to an understanding of the quantum to classical transition[60].

The key concept here is quantum entanglement, where two systems are described by a state that cannot be broken into two individual states for each subsystem. Entangled states encapsulate quantum correlations between the two subsystems. Such correlations embody entirely new physical properties that are not present in the individual subsystems.

Thus, we may say that the systems lost their individuality, and then, the quantum entanglement represents that the whole system is different from the sum of the individual subsystems.

In the quantum picture, the interactions between a system and its environment now have the power to play a much more important role than in classical physics. They will tipically lead to entanglement between the two sub-systems and thus change the nature of the object itself, altering what we may observe at the level of the system.

The coupling with the environment now defines the *coherence*, a measure for the quantumness of the system. There are two main consequences of environmental interactions for a quantum system. The first is the disappearance of quantum coherence and the second one is the selection of a set of robust preferred states for a system.

For example, for a classical ball or any macroscopic object in the presence of an environment, the interaction with photons will not have a non negligible exchange of momentum and thus, these interactions will not change significantly the motion of the ball. Even so, if dissipation is absent, we must not conclude that there is no interaction with the environment, for example, an interaction may not exchange momentum but even so it can lead to a creation of correlation, which induces loss of coherence.

Mathematically, the coherence is viewed as the presence of non diagonal elements in the density matrix. It is clear that once it is defined as basis dependent, knowing what is coherent or not may be a complicated question. For example, in the case of Schrödinger's cat, the natural basis is $\{|alive\rangle, |dead\rangle\}$ because it is this basis that our devices are able to measure.

Dissipation and decoherence are two distinct processes and have distinct time scale. The dissipation is a process of loss of energy and can be observed in classical systems, while the decoherence processes are often viewed as "quantum noises" that sometimes receive the name of *dephasing* [2].

The dephasing processes have been largely studied in the last decades, for spins (or other two level systems), quantum harmonic oscillators, metals and semiconductors, as well for quantum computation [61, 62, 63, 64, 65]. The dephasing noise is a mechanism that, in a

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[2] The dephasing is not the only one that surpresses coherences, but it is one of the most important.

given basis, surpresses all the non-diagonal elements, but does not affect the diagonal ones. As an example [3], let us consider a 2-state system with Hamiltonian $H = \frac{\omega}{2}\sigma_z$, where σ_z is a Pauli matrix [4] and $D(\rho) = \frac{\lambda}{2}\Big(\sigma_z \rho \sigma_z - \rho\Big)$. [5]

In order to compute explicitly $\rho(t)$, we parametrize it in the following way:

$$\rho(t) = \begin{pmatrix} p_+ & q \\ q* & p_- \end{pmatrix}, \tag{5.28}$$

where $p_\pm$ are the probabilities of finding the system at $|\pm\rangle$. [6]

Now we are able to compute each term of the Lindblad equation. Let us begin with the unitary part:

$$i[H,\rho] = i\frac{\omega}{2}\left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} p_+ & q \\ q* & p_- \end{pmatrix} - \begin{pmatrix} p_+ & q \\ q* & p_- \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \tag{5.29}$$

and then

$$i[H,\rho] = i\omega \begin{pmatrix} 0 & q \\ -q* & 0 \end{pmatrix}. \tag{5.30}$$

Now we go further and compute the non-unitary part:

$$D(\rho) = \frac{\lambda}{2}\left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} p_+ & q \\ q* & p_- \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} p_+ & q \\ q* & p_- \end{pmatrix} \right\}, \tag{5.31}$$

which gives us

$$D(\rho) = \lambda \begin{pmatrix} 0 & -q \\ -q* & 0 \end{pmatrix}. \tag{5.32}$$

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[3] This example was taken from a set of lectures of Professor Gabriel Teixeira Landi.

[4] $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

[5] Note that the $D(\rho)$ is in the Lindblad form (Eq.(5.17)) with $L = \sigma_z$. Moreover, note that $\sigma_z^2 = I$

[6] That is the basis of the Hamiltonian.

Therefore, the time evolution of the density matrix is given by

$$\frac{d}{dt}\begin{pmatrix} p_+ & q \\ q* & p_- \end{pmatrix} = \begin{pmatrix} 0 & (-i\omega - \lambda)q \\ (i\omega - \lambda)q* & 0 \end{pmatrix}, \tag{5.33}$$

that gives us the following set of equations:[7]

$$\begin{aligned} \frac{dp_\pm}{dt} &= 0 \\ \frac{dq}{dt} &= (-i\omega - \lambda)q. \end{aligned} \tag{5.34}$$

Then, the diagonal terms are constant and the non-diagonal ones relax toward zero as $t \to \infty$. So, the dephasing noise may be interpreted as a relaxation without exchange of energy, once the populations are constant, in the basis of the Hamiltonian.

Finally, we can note that the Lindblad generator L considered in this example is hermitian and commutes with the Hamiltonian. These facts will be important in the construction of the phenomenological dephasing used in this dissertation.

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[7] Note that solving the equation for $q(t)$, we obtain the solution for $q^*(t)$ taking the complex conjugate of $q(t)$, so we do not have to solve twice.

Chapter 6

Evolution of Two Fermionic 1D Chains Under Dephasing Influence

In chapter 3, we discussed how to treat a problem of a one-dimensional tight-binding chain with N sites. Now we go ahead and take two chains with N sites each.

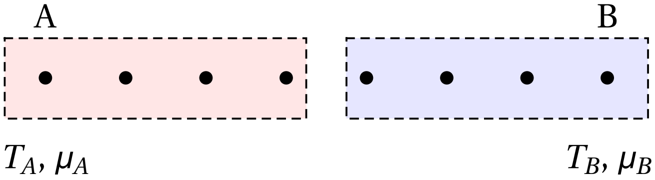

Figure 6.1: Systems A and B initially prepared at different temperatures and chemical potentials.

Consider two one-dimensional systems A and B of N sites each, initially separated and prepared at temperature T_A and T_B and chemical potentials μ_A and μ_B respectively, as shown in figure 6.1. At $t = 0$, the systems are joined by an coupling and we let them evolve.

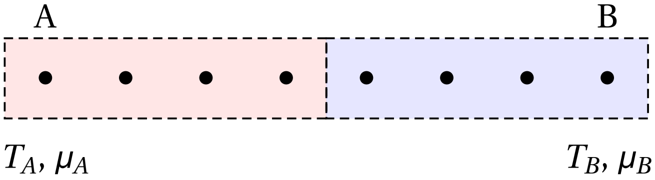

Figure 6.2: Systems A and B initially prepared at different temperatures and chemical potentials.

The Hamiltonian of a unique one-dimensional chain with $2N$ sites with controlable couplings between the sites is:

$$H = \sum_{i=1}^{2N} g_i (c_{i+1}^{\dagger} c_i + c_i^{\dagger} c_{i+1}) \tag{6.1}$$

For this dissertation we will consider that each half is homogeneous, in the aspect that all the couplings have the same value and the coupling between the chains has another value. Then, the Hamiltonian of the full system will be divided as follows:

$$H = H_A + H_B + V. \tag{6.2}$$

The terms H_A and H_B are the Hamiltonians of each part, which corresponds to a simple Hamiltonian of a one-dimensional chain, each one prepared with a given temperature and chemical potentials where V corresponds to the potential of interaction. The H_A and H_B have the same shape and are given by:

$$H_A = -\alpha \sum_{i=1}^{N-1} (c_{i+1}^{\dagger} c_i + c_i^{\dagger} c_{i+1}) \qquad H_B = -\alpha \sum_{i=N}^{2N-1} (c_{i+1}^{\dagger} c_i + c_i^{\dagger} c_{i+1}) \tag{6.3}$$

$$V = g_0 (c_N^{\dagger} c_{N+1} + c_{N+1}^{\dagger} c_N). \tag{6.4}$$

In Sec.(3.3) we showed how to diagonalize a single 1D chain by conveniently choosing a linear combination of the fermionic operators. There a new set of operators was written as a linear combination of the previous set. So, we will consider the same set for one-dimensional chains with open boundary condition as ansatz. Then we will use

$$c_i = \sum_k S_{ik} a_k \tag{6.5}$$

for H_A and

$$c_{i+N} = \sum_k S_{ik} b_k \tag{6.6}$$

for H_B, where $S_{ik} = \sqrt{\frac{2}{N+1}} \sin(ik)$.

For each term with $i \leq N$, we will write c_i in terms of a_k and for $i > N$, we shall write in terms of b_k . Replacing in V:

$$V = g_0 \sum_{k,k'} S_{kN} S_{k'1} a_k^\dagger b_{k'} + S_{kN} S_{k'1} b_{k'}^\dagger a_k \tag{6.7}$$

Replacing the values of S_{ik} in V, we find:

$$V = \frac{2g_0}{N+1} \sum_{k,k'} \sin(Nk)\sin(k')[a_k^\dagger b_{k'} + b_{k'}^\dagger a_k] \tag{6.8}$$

In order to simplify the problem we move to the interaction picture. The potential in this representation is

$$\tilde{V}(t) = e^{iH_0 t} V e^{-iH_0 t} = \sum_{k,k'} G_{k,k'}[e^{i(\epsilon_k - \epsilon_{k'})t} a_k^\dagger b_k + e^{-i(\epsilon_k - \epsilon_{k'})t} b_k^\dagger a_k] \tag{6.9}$$

where $\tilde{V}(t)$ is the potential in the interaction picture and $G_{k,k'} = \frac{2g}{N+1}\sin(Nk)\sin(k')$.

We see that terms with $k \neq k'$ will have rapid oscillations. As it is well known from perturbation theory, if the coupling constants $G_{k,k'}$ are also small, then the rotating terms will have a negligible effect in the dynamics [66]. Hence, in this case, we may retain in the calculations only those terms with $k' = k$. We also note that this approximation has been tested extensively via numerical simulations in Ref.[9]. That is, we approximate the Hamiltonian to

$$H = \sum_k \epsilon_k \left(a_k^\dagger a_k + b_k^\dagger b_k \right) + \frac{g_0}{N+1} \sum_k \sin(Nk)\sin(k)[a_k^\dagger b_k + b_k^\dagger a_k]. \tag{6.10}$$

Writing $\sin(Nk) = (-1)^{l+1}\sin(k)$, the Hamiltonian has the following shape:

$$H = \sum_k \epsilon_k \left(a_k^\dagger a_k + b_k^\dagger b_k \right) + \frac{g_0}{N+1} \sum_k (-1)^{l+1} \sin^2(k)[a_k^\dagger b_k + b_k^\dagger a_k] \tag{6.11}$$

and then

$$H = \sum_k \epsilon_k \left(a_k^\dagger a_k + b_k^\dagger b_k \right) + \sum_k G_k [a_k^\dagger b_k + b_k^\dagger a_k] \tag{6.12}$$

where $G_k = (-1)^{l+1} \frac{g_0}{N+1} \sin^2(k)$.

For each subspace of momentum k, the Hamiltonian is the same as the interaction of a system of two sites. Since the Hamiltonian factorizes, we can work with individual k's which will be an important property that will allow us to analyze separately the probabilities of exchange of particle for each k. To finish the diagonalization, we define a new set of operators. The change of basis will be the same as made in the two sites problem.

$$\eta_{k,\sigma} = \frac{a_k + \sigma b_k}{\sqrt{2}} \tag{6.13}$$

Using the new set we get:

$$H = \sum_{k,\sigma} (\epsilon_k + \sigma G_k) \eta^{\dagger}_{k,\sigma} \eta_{k,\sigma} \tag{6.14}$$

We therefore see that, within this approximation, the system factors into two energy bands with dispersion relations corrected by the factor G_k, which is assumed to be small.

6.1 Lindblad Equation and Phenomenological Dephasing

After diagonalization, we look at the dynamics of the system. After the systems are connected, we can apply a dephasing noise and analyze its influence over the system. In this dissertation we shall use a phenomenological energy conserving noise. The main property we impose is that, the average of the Hamiltonian has to be conserved and to know the conditions in which it occurs, we use

$$\frac{d}{dt}\langle \mathcal{O} \rangle = i \langle [H, \mathcal{O}] \rangle + \gamma \langle \tilde{D}(\mathcal{O}) \rangle. \tag{6.15}$$

Replacing the Hamiltonian in this equation, we see that the unitary part directly vanishes. So, the time evolution of the average of the Hamiltonian is

$$\begin{aligned} \frac{d}{dt}\langle H \rangle &= \gamma \langle \tilde{D}(H) \rangle = 0 \\ &= \gamma \, \langle L^{\dagger} H L - \frac{1}{2}\{L^{\dagger} L, H\} \rangle \\ &= \frac{\gamma}{2} \, \langle L^{\dagger}[H, L] - [H, L^{\dagger}] L \rangle = 0. \end{aligned} \tag{6.16}$$

Thus, basically we have to find a Lindbladian L that satisfies the condition above. To accomplish this task we see that it suffices to choose a set of Lindblad generators which commute with the Hamiltonian.

Using these conditions, I propose a dephasing that acts separately in each subspace of momentum k and type of particle with the following shape:

$$D(\rho)_{k,\pm} = \eta^\dagger_{k,\pm}\eta_{k,\pm}\rho\eta^\dagger_{k,\pm}\eta_{k,\pm} - \frac{1}{2}\Big\{\eta^\dagger_{k,\pm}\eta_{k,\pm}, \rho\Big\}. \tag{6.17}$$

Thus, in a subspace k, the dephasing will be

$$D(\rho)_k = D(\rho)_{k,+} + D(\rho)_{k,+}. \tag{6.18}$$

Evolution of mean values

The objective here is to compute the evolution of the mean values of occupation and energy of the systems. Therefore we shall compute $\langle\eta^\dagger_+\eta_+\rangle$, $\langle\eta^\dagger_-\eta_-\rangle$, $\langle\eta^\dagger_-\eta_+\rangle$ and $\langle\eta^\dagger_+\eta_-\rangle$, where c_i are constants. The terms with the commutators are summarized as follows:

$$\begin{aligned}
\langle[H, \eta^\dagger_+\eta_+]\rangle &= 0 && (6.19)\\
\langle[H, \eta^\dagger_-\eta_-]\rangle &= 0 && (6.20)\\
\langle[H, \eta^\dagger_+\eta_-]\rangle &= 2G_k\langle\eta^\dagger_+\eta_-\rangle && (6.21)\\
\langle[H, \eta^\dagger_-\eta_+]\rangle &= -2G_k\langle\eta^\dagger_-\eta_+\rangle, && (6.22)
\end{aligned}$$

and the terms of the adjoint dissipator are:

$$\begin{aligned}
\langle\tilde{D}(\eta^\dagger_+\eta_+)\rangle &= 0 && (6.23)\\
\langle\tilde{D}(\eta^\dagger_-\eta_-)\rangle &= 0 && (6.24)\\
\langle\tilde{D}(\eta^\dagger_+\eta_-)\rangle &= -\langle\eta^\dagger_+\eta_-\rangle && (6.25)\\
\langle\tilde{D}(\eta^\dagger_-\eta_+)\rangle &= -\langle\eta^\dagger_-\eta_+\rangle. && (6.26)
\end{aligned}$$

Once each term of the equations is determined, we get:

$$\begin{aligned} \frac{d}{dt}\langle \eta_+^\dagger \eta_+ \rangle &= 0 && (6.27)\\ \frac{d}{dt}\langle \eta_-^\dagger \eta_- \rangle &= 0 && (6.28)\\ \frac{d}{dt}\langle \eta_+^\dagger \eta_- \rangle &= (2iG_k - \lambda)\langle \eta_+^\dagger \eta_- \rangle && (6.29)\\ \frac{d}{dt}\langle \eta_-^\dagger \eta_+ \rangle &= (-2iG_k - \lambda)\langle \eta_-^\dagger \eta_+ \rangle. && (6.30)\\ & && (6.31) \end{aligned}$$

These equations give us

$$\begin{aligned} \langle \eta_+^\dagger \eta_+ \rangle &= c_1\\ \langle \eta_-^\dagger \eta_- \rangle &= c_2\\ \langle \eta_+^\dagger \eta_- \rangle &= c_3 e^{(2iG_k - \lambda)t}\\ \langle \eta_-^\dagger \eta_+ \rangle &= c_4 e^{(-2iG_k - \lambda)t}, \end{aligned} \tag{6.32}$$

where c_i are integration constants.

The initial condition is the thermal state for $\langle a_k^\dagger a_k \rangle$ and $\langle b_k^\dagger b_k \rangle$ and zero for $\langle a_k^\dagger b_k \rangle$ and $\langle b_k^\dagger a_k \rangle$ because the systems are initially uncorrelated. Using the results of 6.32, we find:

$$\begin{aligned} \langle a_k^\dagger a_k \rangle_0 &= \frac{1}{2}(c_1 + c_2 + c_3 + c_4) = n_{A,k}\\ \langle b_k^\dagger b_k \rangle_0 &= \frac{1}{2}(c_1 + c_2 - c_3 - c_4) = n_{B,k}\\ \langle a_k^\dagger b_k \rangle_0 &= \frac{1}{2}(c_1 - c_2 - c_3 + c_4) = 0\\ \langle b_k^\dagger a_k \rangle_0 &= \frac{1}{2}(c_1 - c_2 + c_3 - c_4) = 0. \end{aligned} \tag{6.33}$$

From these, we obtain explicity that $c_1 = c_2 = \frac{n_{A,k}+n_{B,k}}{2}$ and $c_3 = c_4 = (\frac{n_{A,k}-n_{B,k}}{2})$. Combining everything, we may finally write the time evolution of the relevant operators as:

$$\langle a_k^\dagger a_k \rangle_t = \frac{n_{a,k} + n_{b,k}}{2} + \Big(\frac{n_{a,k} - n_{b,k}}{2}\Big) e^{-\lambda t} \cos(2G_k t) \tag{6.34}$$

and

$$\langle b_k^\dagger b_k \rangle_t = \frac{n_{a,k} + n_{b,k}}{2} - \Big(\frac{n_{a,k} - n_{b,k}}{2}\Big) e^{-\lambda t} \cos(2G_k t). \tag{6.35}$$

The correlations are given by

$$\langle a_k^\dagger b_k \rangle_t = i\Big(\frac{n_{A,k} - n_{B,k}}{2}\Big) e^{-\lambda t} \sin(2G_k t) \tag{6.36}$$

Then the individual average occupation and the Hamiltonians are given by:

$$\langle N_A \rangle = \sum_k \Bigg(\Bigg(\frac{n_{A,k} + n_{B,k}}{2}\Bigg) + \Bigg(\frac{n_{A,k} - n_{B,k}}{2}\Bigg) e^{-\lambda t} \cos(2G_k t) \Bigg) \tag{6.37}$$

$$\langle N_B \rangle = \sum_k \Bigg(\Bigg(\frac{n_{A,k} + n_{B,k}}{2}\Bigg) - \Bigg(\frac{n_{A,k} - n_{B,k}}{2}\Bigg) e^{-\lambda t} \cos(2G_k t) \Bigg) \tag{6.38}$$

$$\langle H_A \rangle = \sum_k \epsilon_k \Bigg(\Bigg(\frac{n_{A,k} + n_{B,k}}{2}\Bigg) + \Bigg(\frac{n_{A,k} - n_{B,k}}{2}\Bigg) e^{-\lambda t} \cos(2G_k t) \Bigg) \tag{6.39}$$

$$\langle H_B \rangle = \sum_k \epsilon_k \Bigg(\Bigg(\frac{n_{A,k} + n_{B,k}}{2}\Bigg) - \Bigg(\frac{n_{A,k} - n_{B,k}}{2}\Bigg) e^{-\lambda t} \cos(2G_k t) \Bigg) \tag{6.40}$$

With this result, it is possible to see that the chosen form of the dephasing enables the system to thermalize. Note that in the limit of $t \to \infty$, $\langle H_A \rangle = \langle H_B \rangle$, which is the result expected from thermodynamics in the case of thermalization between two identical systems. Moreover, the occupation of each system will be the same as well, in this limit.

6.2 Fluxes and Onsager Coefficients

As previously discussed, a flux is a derivative with respect to time of some extensive parameter. In this dissertation, I will use the Onsager's Theorem in a slightly different way. Since $\langle H_A \rangle_t$ and $\langle N_A \rangle_t$ are already determined in terms of sums, I will define

$$\mathcal{J}_N \equiv \frac{1}{N}(\langle N_A \rangle_t - \langle N_A \rangle_0) \tag{6.41}$$

that has an interpretation of the total quantity of particles per site that flowed through the system B to the system A [1]. The same ideia will be used for the heat. As an abuse of language, I will call these the total quantity that flowed until the time t as *flux*. For example, the total number of particles that flowed until the time t we will call just as *the flux of particles at the time t*. In addition, we also define the total heat flowed until the time t, that will be refered as *the flux of heat at the time t*, by

$$\mathcal{J}_Q = \frac{1}{N}((\langle H_A \rangle_t - \mu \langle N_A \rangle_t) - (\langle H_A \rangle_0 - \mu \langle N_A \rangle_0). \tag{6.42}$$

For two subsystems with temperatures $T_A = T + \frac{\delta T}{2}$ and $T_B = T - \frac{\delta T}{2}$, the fluxes of particle and heat can be expanded in Taylor series in the following way:

$$\begin{aligned} \mathcal{J}_N &= \frac{\partial \mathcal{J}_N}{\partial \mu}\delta\mu + \frac{\partial \mathcal{J}_N}{\partial T}\delta T \\ \mathcal{J}_Q &= \frac{\partial Q}{\partial \mu}\delta\mu + \frac{\partial Q}{\partial T}\delta T. \end{aligned} \tag{6.43}$$

Moreover, I will define $J_{N,\mu} \equiv L'_{11} =$ and $J_{N,T} \equiv L'_{12}$ as the quantity of particles flowed due to a difference of chemical potential and temperature, respectively. We also define

$$\begin{aligned} J_{N,\mu} &\equiv L'_{11} = T\frac{\partial \mathcal{J}_N}{\partial \mu} \\ J_{Q,\mu} &\equiv L'_{21} = T\frac{\partial Q}{\partial \mu} \\ J_{N,T} &\equiv L'_{12} = T^2\frac{\partial \mathcal{J}_N}{\partial T} \\ J_{Q,T} &\equiv L'_{22} = T^2\frac{\partial Q}{\partial T}, \end{aligned} \tag{6.44}$$

and $J_{Q,\mu} \equiv L'_{21}$ and $J_{Q,T} \equiv L'_{22}$ with analog interpretation.

6.2.1 Thermodynamic Limit and Final Fluxes

In this subsection I will treat the fluxes for $t \to \infty$ and $N \to \infty$. The second condition gives us the possibility to treat the occupations and the energies as done in Sec.(3.4.3). It is

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[1] The inverse case can also be determined. Once we have to obey some closure relations, the cases $A \to B$ can be determined just changing the signal of the result.

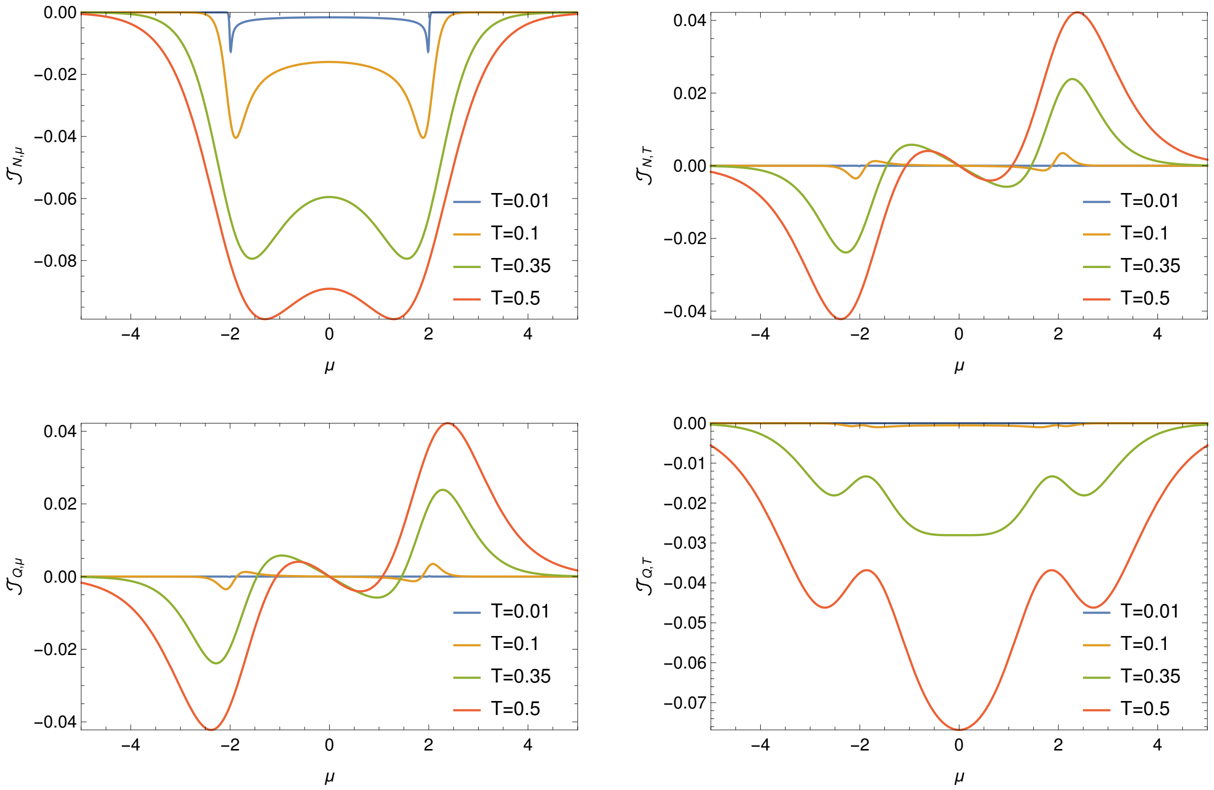

Figure 6.3: Final fluxes per site for $N \to \infty$ for lower temperatures. The temperatures are given in units of α.

clear that the related integrals are very difficult. Here and in the next subsections, the results were obtained using the software *Mathematica*. For the subsection 6.2.4, I dealt with low temperatures and used Sommerfeld expansion in order to find an analytical solution.

As a first thing that we can note in Fig.(6.3-6.4) is that $\mathcal{J}_{N,\mu}$ and $\mathcal{J}_{Q,T}$ are even, while $\mathcal{J}_{N,T}$ and $\mathcal{J}_{Q,\mu}$ are odd with respect to the chemical potential μ. The parity of the fluxes can be explained through the parity of the energy band. Although the interval is not simmetric with relation to $k = 0$, if we take the center of the band, i.e. $k = \frac{\pi}{2}$, the band will be simmetric. In other words, the difference of energy between the lowest level and the next is the same of the highest one and the previous and therefore, we can expect some simmetry of the fluxes.

In Fig.(6.3), we can also see that the fluxes go to zero when $\mu \leq -4$. It occurs because the probability of a level to be occupied is too low, then the probability of a flux occur is low as well. For $\mu \geq 4$, the fluxes are negligible because the probability of a level to be occupied is too high. Due to Pauli's Exclusion Principle, if a level is occupied in both subsystems, no fluxes will occur in this level. These facts can also be seen in Fig.(6.4) for different values of μ. This difference occurs because high temperature compensates the occupation and makes the possibility of having fluxes possible.

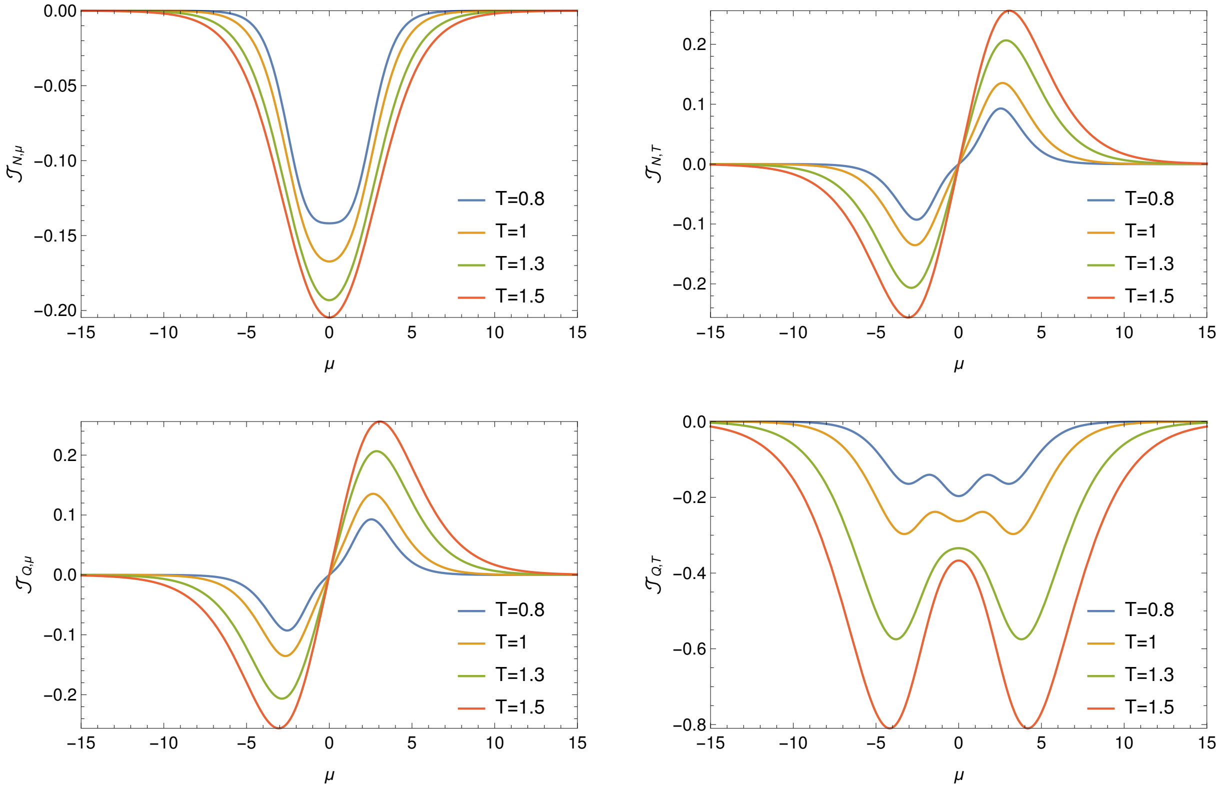

Figure 6.4: Final fluxes per site for $N \to \infty$ for higher temperatures. The temperatures are given in units of α.

Still in figures (6.3) and (6.4), we can see that the fluxes increase with temperature. This also occurs because the disorder of the system increases and the possibilites of exchange of particles and energy increase as well.

The fluxes of energy are directly related to the flux of particles in the following way:

$$\mathcal{J}_{E,k} = \langle H_k(t) \rangle - \langle H_k(0) \rangle = \epsilon_k \mathcal{J}_{N,k} \tag{6.45}$$

where the subindices k tell us that we are dealing with one specific value of k. Since $\mathcal{J}_{Q,k} = (\epsilon_k - \mu)\mathcal{J}_{N,k}$, the flux of heat depends on the competition between the ϵ_k and μ. Particularly, for small temperatures, the heat flux due to a difference of temperature ($\mathcal{J}_{Q,T}$), it takes the maximum intensity for $\mu = 0$. This fact occurs because for $T = 0$, $\mu = 0$ leaves us in the ground state of the system and for low temperatures, the mean occupations are not much different compared with null temperature. Then, any difference of temperature causes a difference of occupation in such a way that will favor the flux. For higher temperatures, the competition between chemical potential and temperatures surpresses such effect.

6.2.2 Final Fluxes for Finite Chains

Now we can go further and analyze the dependence of the fluxes with the number of sites. First, we need to remember that we are dealing with fluxes *per site*.

6.2.2.1 Analysis for Fixed μ

Observing Fig.(6.5) we can notice that the number of sites does not influence the behavior of the fluxes, but has a little influence in the scale.

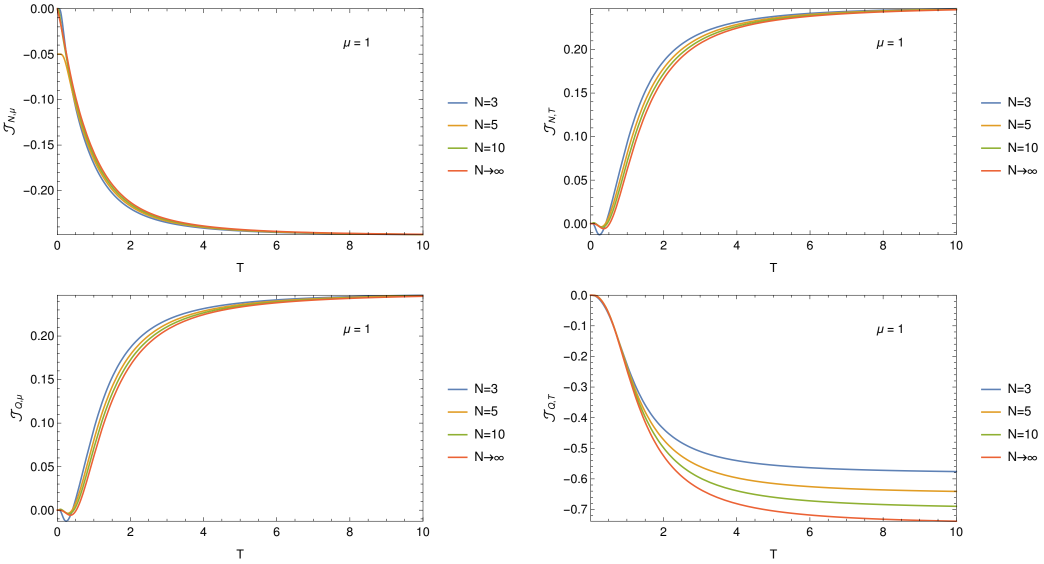

Figure 6.5: Final fluxes for finite chains in a chemical potential μ as a function of temperature. The temperature is given in units of α.

We may also note that there is a kind of "saturation" in the fluxes for very high temperatures. It occurs because the number of states are finite and with higher temperatures, higher occupations occur (for energies above the value of the chemical potential). Since the systems are fermionic, Pauli's Principle of Exclusion has to be obeyed and the fluxes are surpressed.

Finally, the fluxes are a bit different for low temperatures due to the different number of states that are occupied.

6.2.2.2 Analysis for Fixed T

Now we invert the analysis and look at what happens when we fix a temperature T. Only in this subsection, we do not work with fluxes per site. Instead, we consider finite chains, with same lenght and compare the fluxes for the cases with a finite number of sites N and a "infinity" number of sites. This kind of analysis helps us to determine the transition " discrete to continuous analysis".

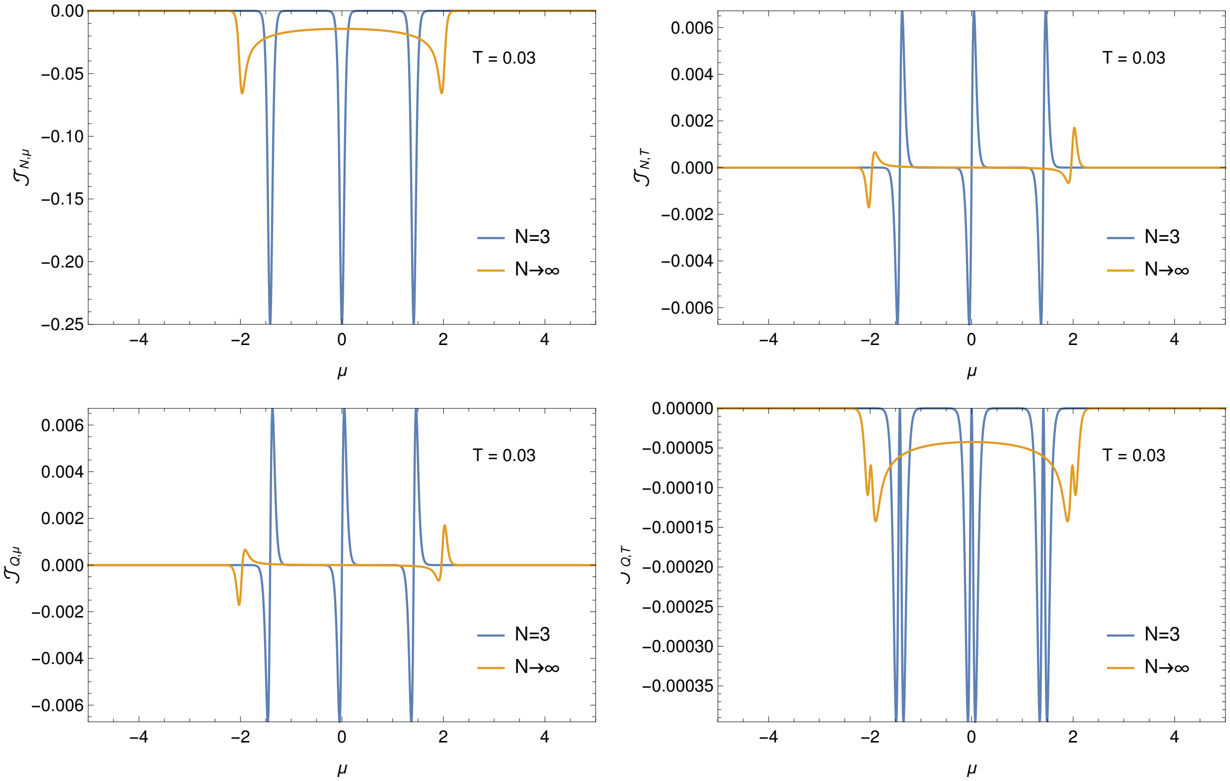

Figure 6.6: Final fluxes for finite chains for a temperature T = 0.01 α, as a function of μ .

We can see in Fig.(6.6- 6.8) that there are some peaks and valleys as the chemical potential is changed. A fact that we can notice is that we have the same numbers of peak/valley and sites. So, for low temperatures, we can explain them using the fact that when we increase the chemical potential, "new" states become available to be occupied. It is clear that allowed set of states is independent of the chemical potential, but its increase makes the states of

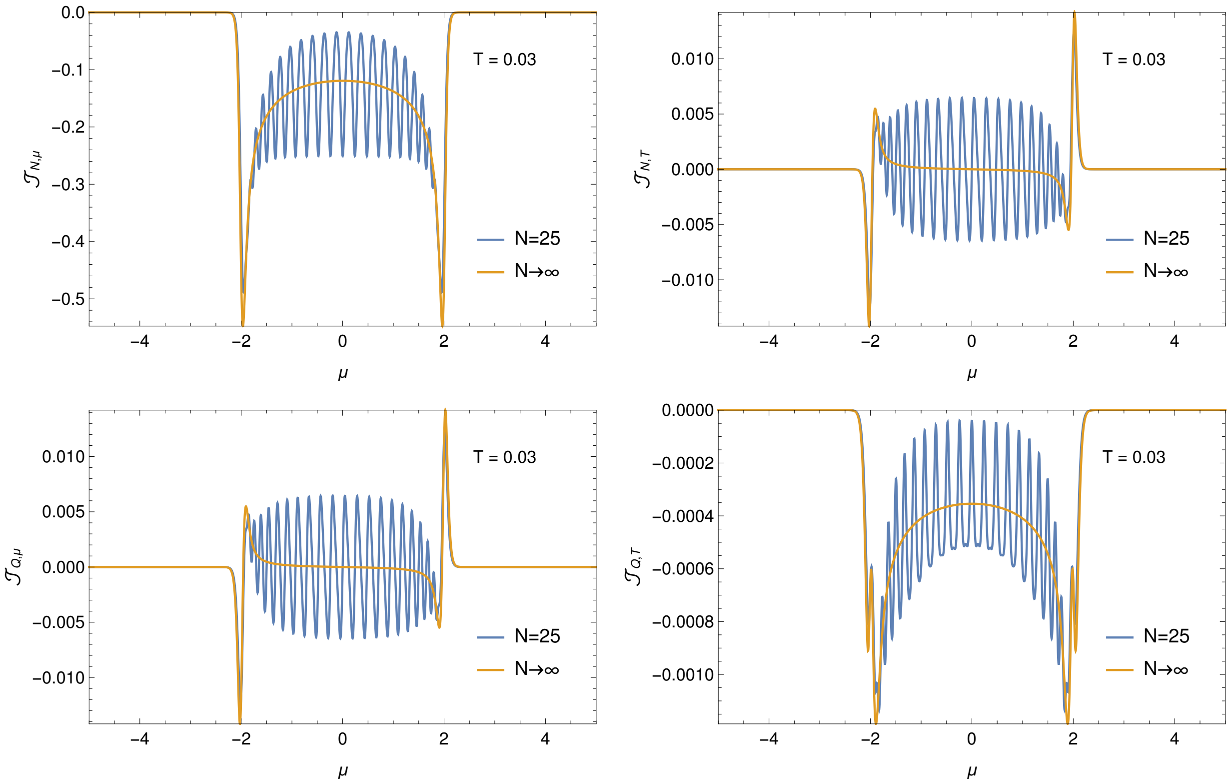

Figure 6.7: Final fluxes for finite chains for a temperature T $= 0.01\ \alpha$, as a function of μ .

more energy more likely to be occupied. Moreover, the intensity of these peaks/valleys can be explained due to the fact that the fluxes studied here are proportional to $\frac{1}{N}$. So, the larger the number of sites is, smaller are the peaks/valleys. Now we can use Fig.(6.8) to analyze the influence of the temperature in these peaks/valleys. As soon as temperature grows, the peaks and valleys becomes softer. It can be explained by using the fact that the temperature smears out the allowed set of states made available by the chemical potential.

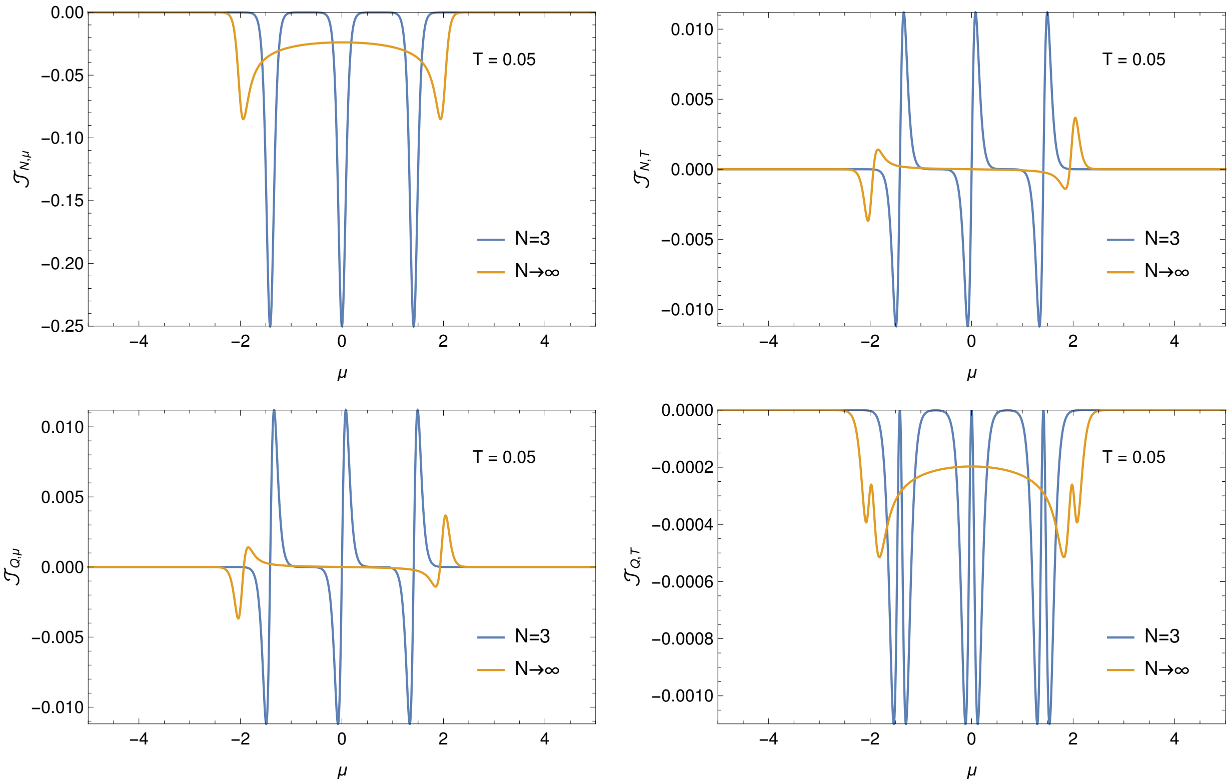

Figure 6.8: Final fluxes for finite chains in a temperature T(in units of α), as function of μ.

6.2.3 Time-Dependent Fluxes

In this subsection I will discuss the time evolution of the fluxes in time. In Fig.(6.10-6.12) we observe the oscilatory behavior of the evolution. This can be explained due to the fact that the particles may be exchanged more than one time. Tendencies of the increase of the flux when we increase the chemical potential can also be observed these figures.

Moreover, in Fig(6.11) we show another point of view of the evolution for different temperatures. These graphics also reinforce the fact analyzed previously that large temperatures also induce large fluxes.

Finally, we also address the typical evolution of the system in the case without dephasing. This problem was studied in [9]. Fig.(6.12) shows the same case of Fig.(6.10) but with no dephasing acting on the systems. In terms of intensity of the fluxes, the dephasing then has no influence. Even so, the dephasing helps the system to thermalize more rapidly.

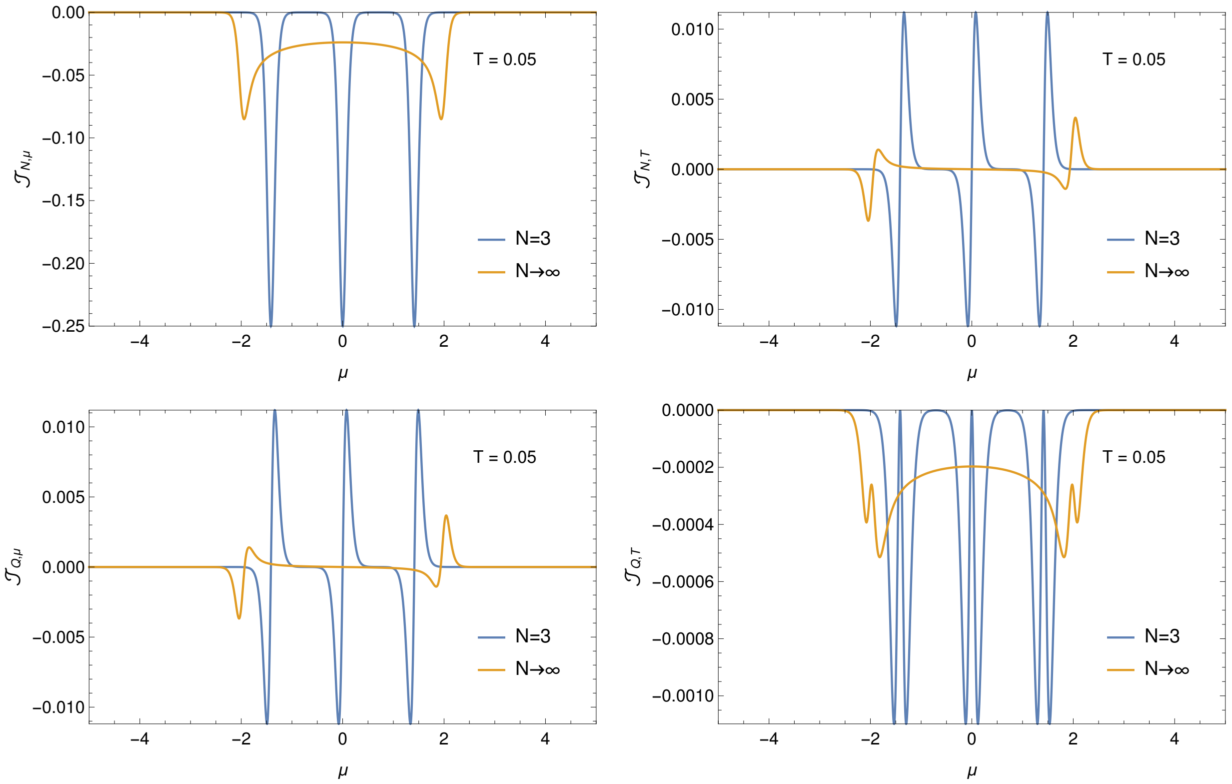

Figure 6.9: Final fluxes for finite chains in a temperature T(in units of α), as function of μ.

6.2.4 Analytical Solution for Low Temperatures

In this section we discuss about the difficulty of obtaining a general analytical solution. Even so it is true, we can obtain an analytical solution for low temperatures using the Sommerfeld expansion. The deduction that I will make below is valid for any two different initial occupations[2], but for the interest of this dissertation, I will consider only small differences for the initial occupations. Moreover, the deductions will be made with the system A as reference, but it can still be made using B as reference.

First, we begin with our definition of the flux of particles

$$\frac{\langle N_A \rangle_t - \langle N_A \rangle_0}{N} = \sum_k \frac{(n_{A,k} - n_{B,k})}{2} \big(e^{-\lambda t}\cos(2G_k t) - 1\big). \tag{6.46}$$

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[2] But they are still at low temperatures

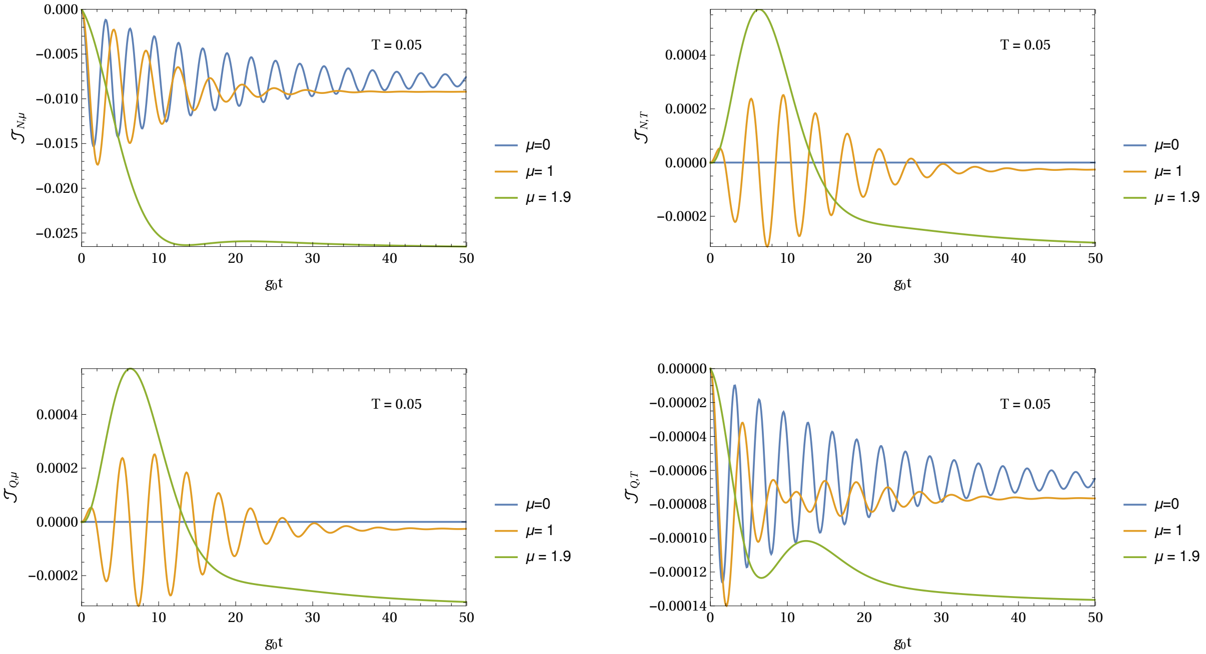

Figure 6.10: Evolution of the fluxes for a fixed temperature and different chemical potentials. The curves correspond to the thermodynamic limit ($N \to \infty$) and $\lambda = 0.05$.

In the thermodynamic limit the sum will be converted into an integral.

$$\begin{aligned} \frac{\langle N_A\rangle_t - \langle N_A\rangle_0}{N} &= \frac{1}{2\pi}\int_0^\pi (n_{A,k}-n_{B,k})(e^{-\lambda t}\cos(2gt\sin^2 k)-1)dk \\ &\equiv \bar{N}_A - \bar{N}_B \qquad (6.47) \end{aligned}$$

where $\bar{N}_X$ is defined by:

$$\bar{N}_X \equiv \frac{1}{2\pi}\int_0^\pi n_{X,k}(e^{-\lambda t}\cos(2gt\sin^2 k)-1)dk \qquad (6.48)$$

with $X = A, B$. The task here then is to find $\bar{N}_X$ and as said before, we will use the Sommerfeld expansion [53] discussed in section (3.4.4). By using it we obtain:

$$\bar{N}_X = \frac{1}{2\pi}\left\{\int_{-2}^{\mu}\frac{(e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4}))-1)}{\sqrt{4-\epsilon^2}}d\epsilon + \frac{\pi^2 T_X^2}{6}\frac{\partial}{\partial\epsilon}\left[\frac{e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4}))-1}{\sqrt{4-\epsilon^2}}\right]_{\epsilon=\mu}\right\} \qquad (6.49)$$

After using the Sommerfeld expansion, the integral may be written once again in k

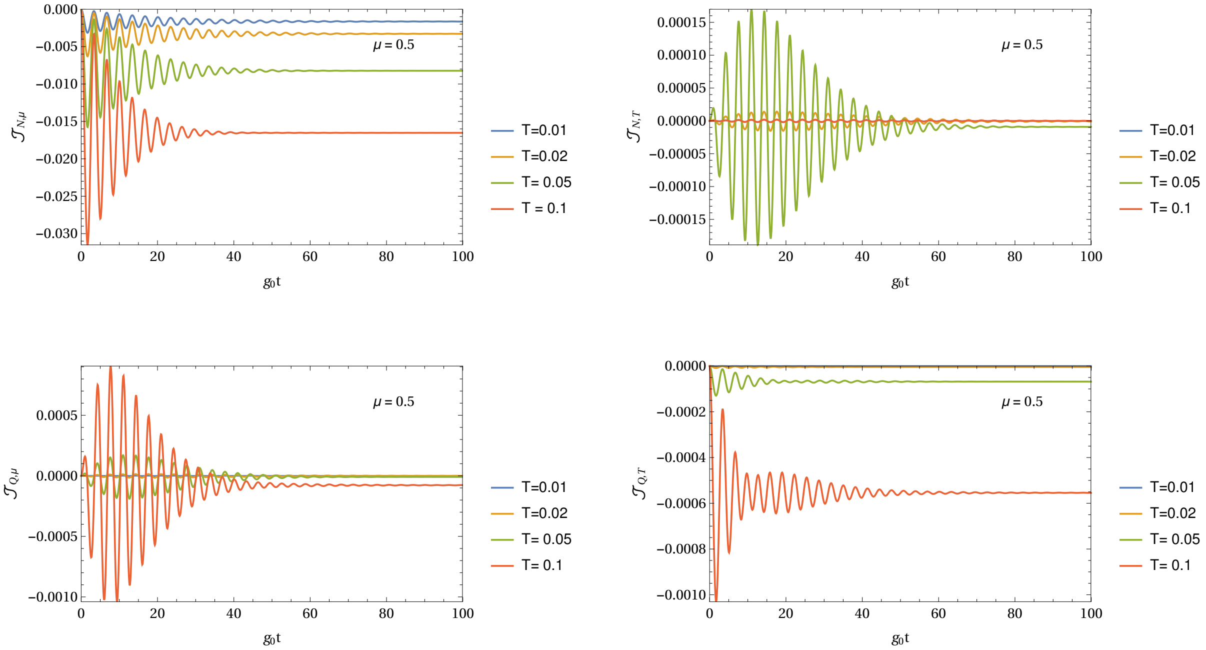

Figure 6.11: Evolution of the fluxes for a fixed chemical potential and different temperatures. The curves correspond to the thermodynamic limit ($N \to \infty$) and $\lambda = 0.05$.

dependence. The only difference between the integral obtained in the beginning and with the expansion is the absence of the occupation $n_{X,k}$ and its upper limit will be changed as $\pi \to \arccos(\frac{-\mu}{2})$. The term related to the derivative can be computed directly and then the main task here is to compute the integral. So, for a moment, let us forget about the second term and let us pay attention to the argument of the integral. The k dependence of the integral is contained in $\cos(2G_k t)$ that can be written as $\cos(gt(1 - \cos(2k)) = \cos(gt)\cos(gt\cos(2k)) + \sin(gt)\sin(gt\cos(2k))$. Since the $\cos(gt)$ and $\sin(gt)$ commute with the integral, the assignment to be done is to compute integrals of $\cos(gt\cos(2k))$ and $\sin(gt\cos(2k))$. In order to solve this, we expand these functions in Bessel functions, as shown in appendix C

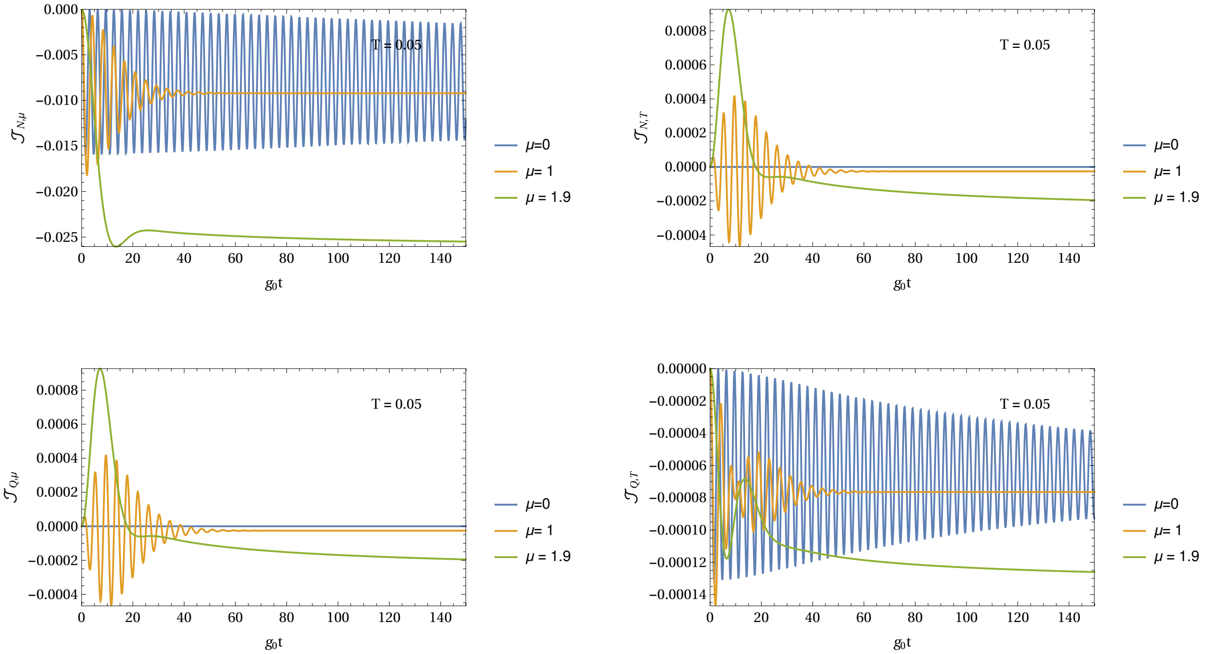

Figure 6.12: Evolution of the fluxes for a fixed temperature and different chemical potentials. The curves correspond to the thermodynamic limit ($N \to \infty$) and $\lambda = 0$.

in Eq.(C.22). Taking $\theta = \Big(2k + \frac{\pi}{2}\Big)$ for the expansion and computing each integral we obtain [3]

$$\begin{aligned}\bar{N}_X &= \frac{1}{2\pi}\Bigg\{e^{-\lambda t}\Big[\cos(gt)\Big(J_0(gt)\arccos(\frac{-\mu}{2}) + \sum_{n=1}^{\infty}(-1)^n\mathcal{W}^{(1)}_{2n}(\mu,gt)\Big) + \sin(gt)\sum_{n=1}^{\infty}(-1)^n\mathcal{W}^{(1)}_{2n-1}(\mu,gt)\Big] \\ &+ \frac{\pi^2T^2\mu}{6}\Big[\frac{e^{-\lambda t}\cos(2gt(1-\frac{\mu^2}{4}))-1}{(4-\mu^2)^{3/2}} + \frac{2gte^{-\lambda t}\sin(2gt(1-\frac{\mu^2}{4}))}{\sqrt{4-\mu^2}}\Big] - \arccos(\frac{-\mu}{2})\Bigg\},\end{aligned} \tag{6.50}$$

in which

$$\mathcal{W}^{(1)}_n(\mu,gt) = \frac{J_n(gt)}{2n}\sin(2n\arccos(\frac{-\mu}{2})). \tag{6.51}$$

So, once we have $\bar{N}_X$, we are able to make the difference of $\bar{N}_A$ and $\bar{N}_B$ to obtain the flux of particles. The approach that allowed us the achievement of the analytical solution did not give us any restriction of initial chemical potentials, but gave us the restriction of the low temperatures. For the interest of this dissertation, we will still use the small difference of

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[3] These calculus are made in details in Appendix (D)

temperature and chemical potential as well. The fluxes $\mathcal{J}_{N,T}$ and $\mathcal{J}_{N,\mu}$ are obtained taking the derivative of $\bar{N}_X$ with respect to the temperatures and chemical potential. The explicit formula will not be shown due to their sizes and no clear physical significance for each separated term.

In the same way that we can obtain analytical solutions for the flux of particles, we can now use the same techniques in order to obtain these solutions for the flux of energy.

Then we start with:

$$\frac{\langle H_A\rangle_t - \langle H_A\rangle_0}{N} = \sum_k \epsilon_k \frac{(n_{A,k} - n_{B,k})}{2}(e^{-\lambda t}\cos(2G_k t) - 1)\Big) \tag{6.52}$$

which can be converted into an integral in the thermodynamic limit.

$$\begin{aligned} \frac{\langle H_A\rangle_t - \langle H_A\rangle_0}{N} &= \frac{1}{2\pi}\int_0^\pi \epsilon_k (n_{A,k} - n_{B,k})(e^{-\lambda t}\cos(2gt\sin^2 k) - 1)dk \\ &\equiv \bar{E}_A - \bar{E}_B \end{aligned} \tag{6.53}$$

where $\bar{E}_X$ is defined by:

$$\bar{E}_X \equiv \frac{1}{2\pi}\int_0^\pi \epsilon_k n_{X,k}(e^{-\lambda t}\cos(2gt\sin^2 k) - 1)dk \tag{6.54}$$

with X defined in the same way did previously. As did before, using the Sommerfeld expansion and solving the integrals, we obtain:

$$\begin{aligned} \bar{E}_X &= \frac{1}{2\pi}\Bigg\{\sqrt{4-\mu^2} + \frac{\pi^2 T^2}{6}\Big[\frac{e^{-\lambda t} gt\mu \sin(2gt(1-\frac{\mu^2}{4})) + e^{-\lambda t}\cos(2gt(1-\frac{\mu^2}{4})) - 1}{\sqrt{4-\mu^2}} + \\ &+ \frac{\mu^2 e^{-\lambda t}\cos(2gt(1-\frac{\mu^2}{4})) - \mu^2}{(4-\mu^2)^{3/2}}\Big] + e^{-\lambda t}\Bigg[\cos(gt)\Big(J_0(gt)\sqrt{4-\mu^2} + \\ &+ 2\sum_{n=1}^{\infty}(-1)^n \mathcal{W}^{(2)}_{2n}(\mu, gt)\Big]\Big) - \sin(gt)\Big(2\sum_{n=1}^{\infty}(-1)^n \mathcal{W}^{(2)}_{2n-1}(\mu, gt)\Big]\Big)\Bigg]\Bigg\}. \end{aligned} \tag{6.55}$$

where I defined

$$\mathcal{W}_n^{(2)}(\mu, gt) = J_n(gt)(\frac{\sin((2n+1)\arccos(\frac{-\mu}{2}))}{2n+1} + \frac{\sin((2n-1)\arccos(\frac{-\mu}{2}))}{2n-1}). \tag{6.56}$$

The fluxes of energy due to difference of chemical potential and temperature are given just taking the derivatives with respect to μ and T. Again, each term of the fluxes has no clear physical interpretation, so they will stay implicit in the result above.

The interval in which the analytical solutions are valid is shown in appendix D.3 for many values of μ.

Chapter 7

Entropy Dynamics and Heat fluctuations

7.1 Density Matrices

In section 6.1 the evolution of averages with the resource of the adjoint dissipator was computed, but as discussed, it is not the unique way to compute averages. If one knows the density matrix, the average of an operator $\mathcal{O}$ is just $\mathrm{tr}(\mathcal{O}\rho)$. But the density matrix is not only useful for computing averages: with it in hand we are able to know the probabilities of finding the system in a given state that is important for finding the fluctuation theorems and heat distributions, as we will see later.

Then, the goal here is to determine the density matrix. Since the dynamics of different k's factorizes, we will solve the Lindblad equation for the subspaces k. The dephasing considered in this problem will be the same used in 6.1.

Albeit the dynamics of the subsystems A and B the Hamiltonian is a priori in the basis of a,b's (with a more clear physical meaning), the calculus in this basis with this dephasing is not short, so for praticity, the evolution of the density matrix will be computed a priori in the basis of η_k's.

The basis is then defined through the number of particles in each state η_+ and η_-. The vacuum state will be denoted as $|1\rangle$ and the other elements will be defined by successive applications of the creation operators onto $|1\rangle$.

$$\begin{aligned} &|1\rangle && (7.1)\\ |2\rangle &= \eta^{\dagger}_{k,+}|1\rangle && (7.2)\\ |3\rangle &= \eta^{\dagger}_{k,-}|1\rangle && (7.3)\\ |4\rangle &= \eta^{\dagger}_{k,+}\eta^{\dagger}_{k,-}|1\rangle && (7.4)\end{aligned}$$

The elements $\rho_{k,ij}$, where $i, j = 1, 2, 3, 4$, are basically $\langle i|\,\rho_k\,|j\rangle$. To determine the evolution of the total density matrix, it is only necessary to compute the evolution element by element of the ρ_k. Therefore, we compute $\langle i|\,[H,\rho]\,|j\rangle$ and $\langle i|\,D(\rho)\,|j\rangle$ one by one.

Remembering that the diagonalized Hamiltonian is

$$H = (\epsilon_k + G_k)\eta^{\dagger}_{k,+}\eta_{k,+} + (\epsilon_k - G_k)\eta^{\dagger}_{k,-}\eta_{k,-}, \tag{7.5}$$

$$\begin{aligned} \frac{d\rho_{11}}{dt} &= 0\\ \frac{d\rho_{12}}{dt} &= \rho_{12}(i(\epsilon_k + G_k) - \frac{\lambda}{2})\\ \frac{d\rho_{13}}{dt} &= \rho_{13}(i(\epsilon_k - G_k) - \frac{\lambda}{2})\\ \frac{d\rho_{14}}{dt} &= \rho_{14}(i2\epsilon_k - \lambda) && (7.6)\end{aligned}$$

$$\begin{aligned} \frac{d\rho_{21}}{dt} &= \rho_{21}(-i(\epsilon_k + G_k) - \frac{\lambda}{2}) && (7.7)\\ \frac{d\rho_{22}}{dt} &= 0 && (7.8)\\ \frac{d\rho_{23}}{dt} &= \rho_{23}(-i2G_k - \lambda) && (7.9)\\ \frac{d\rho_{24}}{dt} &= \rho_{24}(i(\epsilon_k - G_k) - \frac{\lambda}{2}). && (7.10)\end{aligned}$$

We then get:

$$\begin{aligned}
\frac{d\rho_{31}}{dt} &= \rho_{31}(-i(\epsilon_k + G_k) - \frac{\lambda}{2}) \\
\frac{d\rho_{32}}{dt} &= \rho_{32}(2ig_0 - \lambda) \\
\frac{d\rho_{33}}{dt} &= 0 \\
\frac{d\rho_{34}}{dt} &= \rho_{34}(i(\epsilon_k + G_k) - \frac{\lambda}{2})
\end{aligned} \tag{7.11}$$

$$\begin{aligned}
\frac{d\rho_{41}}{dt} &= \rho_{41}(-2i\epsilon_k - \lambda) \\
\frac{d\rho_{42}}{dt} &= \rho_{42}(-i(\epsilon_k - G_k) - \frac{\lambda}{2}) \\
\frac{d\rho_{43}}{dt} &= \rho_{43}(-i(\epsilon_k + G_k) - \frac{\lambda}{2}) \\
\frac{d\rho_{44}}{dt} &= 0
\end{aligned} \tag{7.12}$$

The set above show all of the differential equations that will determine the evolution of each element of the density matrix. Solving all of them, one can obtain:

$$\rho_{\eta,k}(t) = \begin{pmatrix}
c_{11} & c_{12}e^{(iE_+ - \frac{\lambda}{2})t} & c_{13}e^{(iE_- - \frac{\lambda}{2})t} & c_{14}e^{(i2\epsilon_k - \lambda)t} \\
c_{21}e^{(-iE_+ - \frac{\lambda}{2})t} & c_{22} & c_{23}e^{(-2ig_0 - \lambda)t} & c_{24}e^{(iE_- - \frac{\lambda}{2})t} \\
c_{31}e^{(-iE_- - \frac{\lambda}{2})t} & c_{32}e^{(2ig_0 - \lambda)t} & c_{33} & c_{34}e^{(iE_+ - \frac{\lambda}{2})t} \\
c_{41}e^{(-2i\epsilon_k - \lambda)t} & c_{42}e^{(-iE_- - \frac{\lambda}{2})t} & c_{43}e^{(-iE_+ - \frac{\lambda}{2})t} & c_{44}
\end{pmatrix} \tag{7.13}$$

The coeficients c_{ij} are fully determined using the initial conditions of the system. Using the thermal equilibrium as initial condition and transforming to the basis of a's and b's we obtain:

$$\rho_k(t) = \begin{pmatrix} n_{A,k}.n_{B,k} & 0 & 0 & 0 \\ 0 & p_{+,k} & q_k & 0 \\ 0 & q_k* & p_{-,k} & 0 \\ 0 & 0 & 0 & h_{A,k}h_{B,k} \end{pmatrix} \tag{7.14}$$

where

$$q_k = \frac{i}{2}e^{-\lambda t}\sin(2G_k t)(n_{A,k} - n_{B,k}) \tag{7.15}$$

$$p_{\pm,k} = \frac{n_{A,k}h_{B,k} + n_{B,k}h_{A,k}}{2} \pm \frac{e^{-\lambda t}}{2}\cos(2G_k t)(n_{A,k} - n_{B,k}) \tag{7.16}$$

We can also write $p_\pm$ in terms of the evolution of some averages as follows:

$$p_{+,k} = n_{A,k}n_{B,k} + \langle a_k^\dagger a_k \rangle_t. \tag{7.17}$$

$$p_{-,k} = n_{A,k}n_{B,k} + \langle b_k^\dagger b_k \rangle_t. \tag{7.18}$$

and

$$q_k = \langle a_k^\dagger b_k \rangle\,. \tag{7.19}$$

Moreover, we defined $h_{X,k} \equiv (1 - n_{X,k})$, with $X = A, B$.

In the next section, we will need to have in hand the reduced density matrices for the halves A and B in order to analyze the evolution of the individual entropies. In the subspace of the system A, we can write $\rho_{A,k}$ as the following combination:

$$\rho_{A,k}(t) = C_1 I + C_2 a_k + C_3 a_k^\dagger + C_4 a_k^\dagger a_k \tag{7.20}$$

and thanks to Pauli's Exclusion Principle, any higher order terms are identically null. The reduced density matrix may be written as:

$$\rho_{A,k}(t) = 1 - \langle a_k^\dagger a_k \rangle_t + (2\langle a_k^\dagger a_k \rangle_t - 1)a_k^\dagger a_k \tag{7.21}$$

with analogue form for the chain B. Both reduced density matrices are explicitly written as:

$$\rho_{A_k}(t) = \begin{pmatrix} 1 - \langle a_k^\dagger a_k \rangle_t & 0 \\ 0 & \langle a_k^\dagger a_k \rangle_t \end{pmatrix} \qquad \rho_{B_k}(t) = \begin{pmatrix} 1 - \langle b_k^\dagger b_k \rangle_t & 0 \\ 0 & \langle b_k^\dagger b_k \rangle_t \end{pmatrix}. \tag{7.22}$$

7.2 Entropies and Mutual Information

7.2.1 Entropies for the individual chains

Having in hand the density matrices, the eigenvalues give us the probabilities associated with each occupation. As seen in section 7.1, the density matrices ρ_{a_k} and ρ_{b_k} are already diagonal, and the probabilities are the eigenvalues of the density matrices, so it is easy to know what the probabilities are.

Since

$$S = -\mathrm{tr}\{\rho \ln \rho\}, \tag{7.23}$$

then we obtain straightly

$$S_A(t) = -\langle a_k^\dagger a_k \rangle_t \ln(\langle a_k^\dagger a_k \rangle) - (1 - \langle a_k^\dagger a_k \rangle_t) \ln(1 - \langle a_k^\dagger a_k \rangle_t) \tag{7.24}$$

and similarly

$$S_B(t) = -\langle b_k^\dagger b_k \rangle_t \ln(\langle b_k^\dagger b_k \rangle) - (1 - \langle b_k^\dagger b_k \rangle_t) \ln(1 - \langle b_k^\dagger b_k \rangle_t) \tag{7.25}$$

where the occupations are

$$\langle a_k^\dagger a_k \rangle = \left(\frac{n_{A,k} + n_{B,k}}{2} \right) + \left(\frac{n_{A,k} - n_{B,k}}{2} \right) e^{-\lambda t} \cos(2G_k t) \tag{7.26}$$

$$\langle b_k^\dagger b_k \rangle = \left(\frac{n_{A,k} + n_{B,k}}{2} \right) - \left(\frac{n_{A,k} - n_{B,k}}{2} \right) e^{-\lambda t} \cos(2G_k t) \tag{7.27}$$

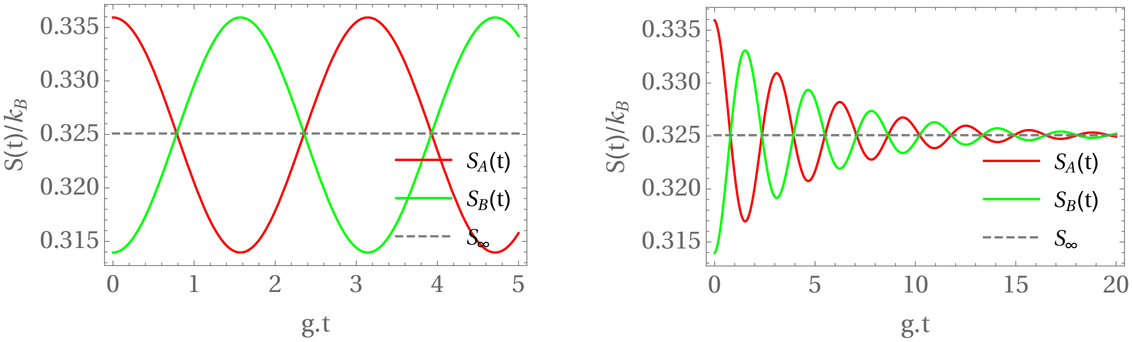
as shown before. Using again $n_{A,k} = n_k + \frac{\delta n}{2}$ and $n_{A,k} = n_k - \frac{\delta n}{2}$ we can expand the entropies in Taylor series . Making it until the second order we get

$$\begin{aligned} S_{A,k}(t) &= -(1-n_k)\ln(1-n_k) - n_k\ln(n_k) + \frac{1}{2}e^{-\lambda t}\cos(2G_k t)\Big(\ln(1-n_k)-\ln(n_k)\Big)\delta n_k \\ &+\frac{e^{-2\lambda t}\cos^2(2G_k t)}{8(n_k-1)n_k}\delta n_k^2 \end{aligned} \tag{7.28}$$

and

$$\begin{aligned} S_{B,k}(t) &= -(1-n_k)\ln(1-n_k) - n_k\ln(n_k) - \frac{1}{2}e^{-\lambda t}\cos(2G_k t)\Big(\ln(1-n_k)-\ln(n_k)\Big)\delta n_k \\ &+\frac{e^{-2\lambda t}\cos^2(2G_k t)}{8(n_k-1)n_k}\delta n_k^2. \end{aligned} \tag{7.29}$$

The term independent of δn_k is exactly the value of the entropy of equilibrium, what is intuitive because the equilibrium will occur with ocupation n_k and the first order in δn_k term means the quantity of entropy exchanged.



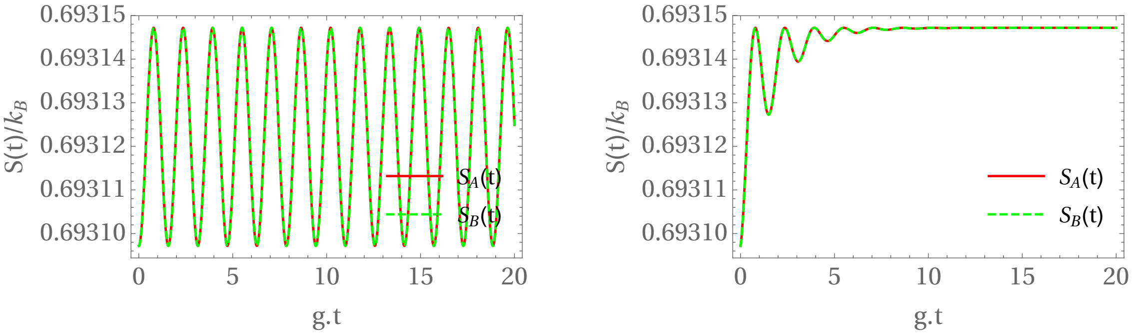
(a) $\lambda = 0$

(b) $\lambda = 0.2$

Figure 7.1: Entropic dynamics for the systems prepared with $n_k = 0.1, \delta n_k = 0.01, g = 1$.

In Fig.(7.1) it is already possible to note the role of damping of the dephasing. For systems with the dephasing some entropy is produced and it is clearer for the case with dephasing shown in 7.2. Finally, as analytically expected, the final entropies converge.

Moreover, as it can be seen in Fig.(7.3), the difference of states do not interfere in the equilibrium state, it interferes only in the evolution.



(a) $\lambda = 0$ (b) $\lambda = 0.2$

Figure 7.2: Entropic dynamics for the systems prepared with $n_k = 0.5, \delta n = 0.01, g = 1$.

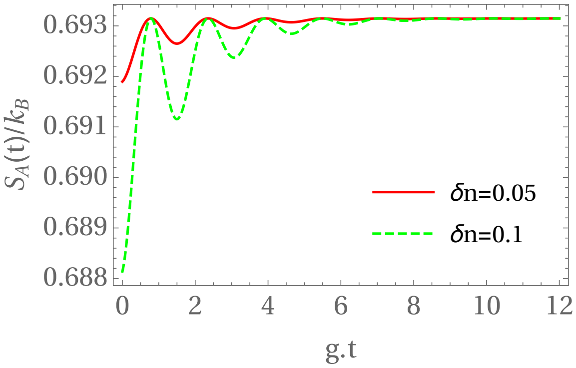


Figure 7.3: Evolution for S_A, with the systems prepared at $n_k = 0.5, g = 1$ and two values $\delta n = 0.05$ and $\delta n = 0.1$

7.2.2 Entropy of the Total System for a Momentum k

As discussed before, the total entropy of the system is not just the sum of the individual entropies. Using the eq. 7.23, we are able to compute the evolution of the total entropy of the system. Through the eigenvalues of the density matrix, the entropy of the total system is

$$\begin{aligned}
S_{AB,k}(t) \;=\; & -(-1+n_{A,k})(-1+n_{B,k})\ln[(-1+n_{A,k})(-1+n_{B,k})] - n_{A,k}n_{B,k}\ln[n_{A,k}n_{B,k}] + \\
& -\frac{1}{2}\left(\langle a_k^\dagger a_k\rangle_t + \langle b_k^\dagger b_k\rangle_k - \sqrt{(\langle a_k^\dagger a_k\rangle_t - \langle b_k^\dagger b_k\rangle_t)^2 + \langle a_k^\dagger b_k\rangle_t \langle b_k^\dagger a_k\rangle_t (n_{A,k}-n_{B,k})^2} \right) \times \\
& \times \ln\left(\langle a_k^\dagger a_k\rangle_t + \langle b_k^\dagger b_k\rangle_k - \sqrt{(\langle a_k^\dagger a_k\rangle_t \langle b_k^\dagger b_k\rangle_t)^2 + \langle a_k^\dagger b_k\rangle_t \langle b_k^\dagger a_k\rangle_t (n_{A,k}-n_{B,k})^2} \right) + \\
& -\frac{1}{2}\left(\langle a_k^\dagger a_k\rangle_t + \langle b_k^\dagger b_k\rangle_k + \sqrt{(\langle a_k^\dagger a_k\rangle_t - \langle b_k^\dagger b_k\rangle_t)^2 + \langle a_k^\dagger b_k\rangle_t \langle b_k^\dagger a_k\rangle_t (n_{A,k}-n_{B,k})^2} \right) \times \\
& \times \ln\left(\langle a_k^\dagger a_k\rangle_t + \langle b_k^\dagger b_k\rangle_k + \sqrt{(\langle a_k^\dagger a_k\rangle_t \langle b_k^\dagger b_k\rangle_t)^2 + \langle a_k^\dagger b_k\rangle_t \langle b_k^\dagger a_k\rangle_t (n_{A,k}-n_{B,k})^2} \right).
\end{aligned} \tag{7.30}$$

This extensive result is the analytical one and it contains no approximation. For δn_k small we can expand in Taylor series one more time, obtaining then:

$$\begin{aligned}
S_{AB,k}(t) \;=\; & -(-1+n_k)^2\ln[(-1+n_k)^2] + 2n_k\Big[(-1+n_k)\ln[-(-1+n_k)n_k] - n_k\ln(n_k)\Big] + \\
& +\frac{1}{4}\left(\frac{e^{-2\lambda t}}{n_k(n_k-1)} + \ln[(-1+n_k)^2]\right)\delta n_k^2
\end{aligned} \tag{7.31}$$

The first term is the final entropy of the total system. Since the occupations will be in equilibrium for a long time, entropy will be as well. From the δn_k^2 we are able to analyze the entropy production of the total system.

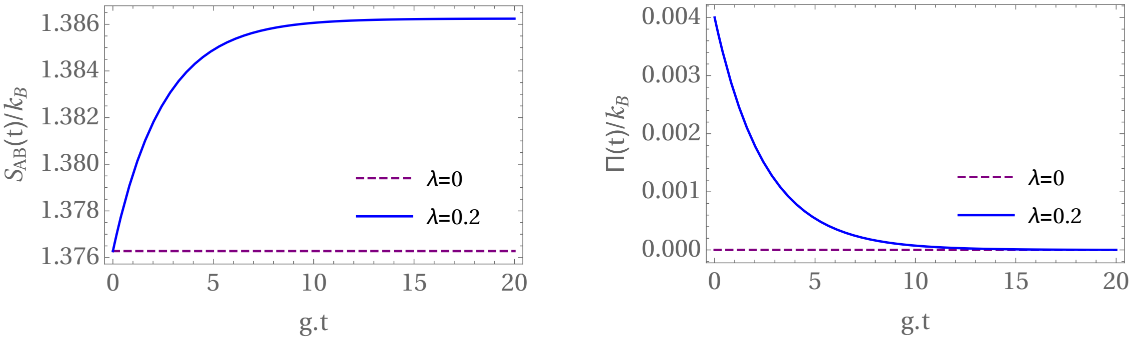
The production rate of entropy is defined as

$$\Pi(t) = \frac{dS_{AB}}{dt}. \tag{7.32}$$

From the equation 7.31 we obtain

$$\Pi(t) = \frac{1}{2}\frac{\lambda e^{-2\lambda t}}{(1-n_k)n_k}\delta n_k^2, \tag{7.33}$$

that is clearly positive. One important thing is that the production is not only positive, but it is non null only for systems under the influence of a dephasing, as it can be seen from the dependence of Π on λ and in the Fig.(7.4).



(a) Total entropy of the system

(b) Entropy production

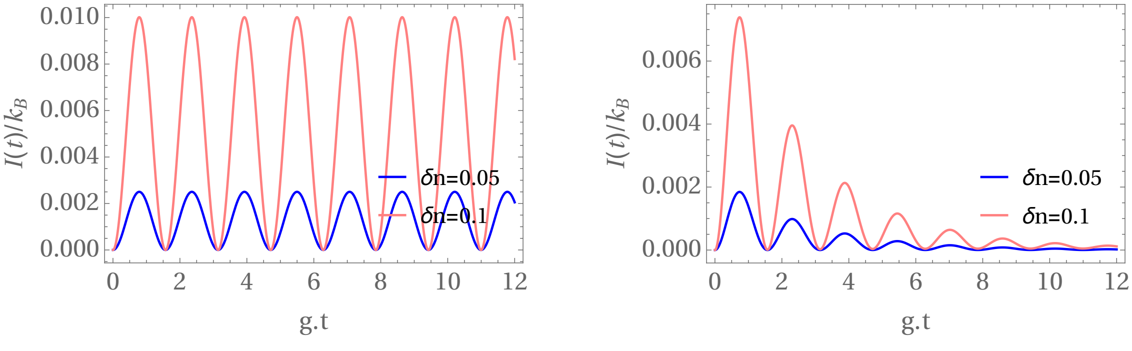
Figure 7.4: Systems prepared with $n_k = 0.5, \delta n = 0.1, g = 1$.

7.2.3 Mutual Information

As discussed before, the mutual information measures how correlated two systems are. Initially we expect the mutual information to be null, since the systems start the dynamics uncoupled.

Using the definition of mutual information and expanding in Taylor series again we find

$$\mathcal{I}(t) = \frac{e^{-2\lambda t}\sin^2(2G_k t)}{4n_k(1-n_k)}\delta n_k^2. \tag{7.34}$$



(a) Evolution of the mutual information in the absence of dephasing.

(b) Evolution of the mutual information in the presence of a dephasing of $\lambda = 0.2$.

Figure 7.5: Systems prepared with $n_k = 0.5, g = 1$.

Then, it is possible to see that the mutual information shows that the systems begin in fact uncorrelated and they start to correlate as time flows and after some instants, the correlation begins to decay periodically, until it gets zero, that is the thermal equilibrium.

7.3 Exchange Probability for a Momentum k

Thanks to the weak coupling we were able to decouple the different momenta dependence, in other words, the creation of a particle with momentum k in a chain has no influence on the destruction of a particle with momentum k' of the another chain and vice versa. So, the processes of exchange of energy are related to the exchange of particles. Thus, if there are no particles in both chains for a certain value of momentum, then we expect that this level will not contribute to the exchange of energy. In the case where a certain momentum k is occupied in both chains, due to the Pauli Exclusion Principle, then we will not have an exchange of energy either.

Therefore, the cases that will have exchange of energy are only the ones when there is one particle with momentum k in a chain and no particles in the other chain in the same state. These idea are also shown in figure 7.6.

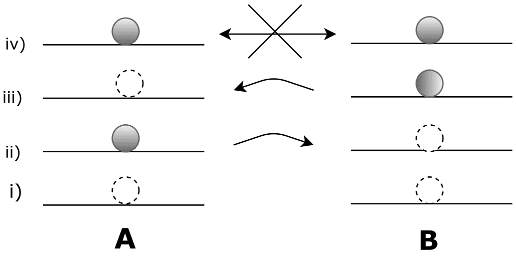


Figure 7.6: The four possibilities for a momentum k. i) There are no particles in the chain A, as well as in chain B, ii)Chain A with one particle and B with no particles. Exchange is allowed, iii)Chain B with one particle and A with no particles. Exchange is allowed, iv) There is one particle in each chain. Therefore, there are no exchanges.

The states $|A, B\rangle$, where A and B can be only zero or one, explicity tells us the number of particles in each chain for a state of momentum and are defined as:

$$|0,0\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad |1,0\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \quad |0,1\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad |1,1\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \tag{7.35}$$

For a given momentum, the probability of a system exchange a heat Q_k is given by

$$P(Q_k) = \sum_{n,m} \langle m|\, \rho(t)\, |m\rangle \langle n|\, \rho_0\, |n\rangle\, \delta(Q - (E_m - E_n)), \tag{7.36}$$

where n and m can be any of the states given by 7.35 , the term $\langle n|\, \rho_0\, |n\rangle$ gives the probability of finding the system in the state n and the term $\langle m|\, \rho_n(t)\, |m\rangle$ is the probability of finding the sytem in m given the initial state n.

Once we measure the system, the state colapse to one of 7.35. The possibilities of initial density matrix ρ_0 are

$$\rho_1 = \begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}, \quad \rho_2 = \begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix} \quad \rho_3 = \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&1&0\\0&0&0&0\end{pmatrix} \quad \rho_4 = \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{pmatrix}, \tag{7.37}$$

where ρ_1, ρ_2, ρ_3, ρ_4 are referred to the initial states $|0,0\rangle$, $|1,0\rangle$,$|0,1\rangle$ and $|1,1\rangle$ respectively.

Using the software *Mathematica* to solve the Lindblad equation for each initial state, we get

$$\rho_1 = \begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}, \qquad \rho_2 = \begin{pmatrix}0&0&0&0\\0&\frac{1}{2}(1+e^{-\lambda t}cos(2G_k t))&\frac{1}{2}ie^{-\lambda t}sin(2G_k t)&0\\0&-\frac{1}{2}ie^{-\lambda t}sin(2G_k t)&\frac{1}{2}(1-e^{-\lambda t}cos(2G_k t))&0\\0&0&0&0\end{pmatrix} \tag{7.38}$$

and

$$\rho_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2}(1 - e^{-\lambda t} cos(2G_k t)) & -\frac{1}{2} i e^{-\lambda t} sin(2G_k t) & 0 \\ 0 & \frac{1}{2} i e^{-\lambda t} sin(2G_k t) & \frac{1}{2}(1 + e^{-\lambda t} cos(2G_k t)) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \rho_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{7.39}$$

As expected, the state without particles and the state totally occupied do not evolve, because the number of particles is conserved and the Pauli Exclusion Principle is obeyed. The states with one particle are initially uncorrelated but as soon as the systems A and B interact, these states will be correlated. This correlation vanishes by the action of the dephasing, that for a long time will make both states equally likely.

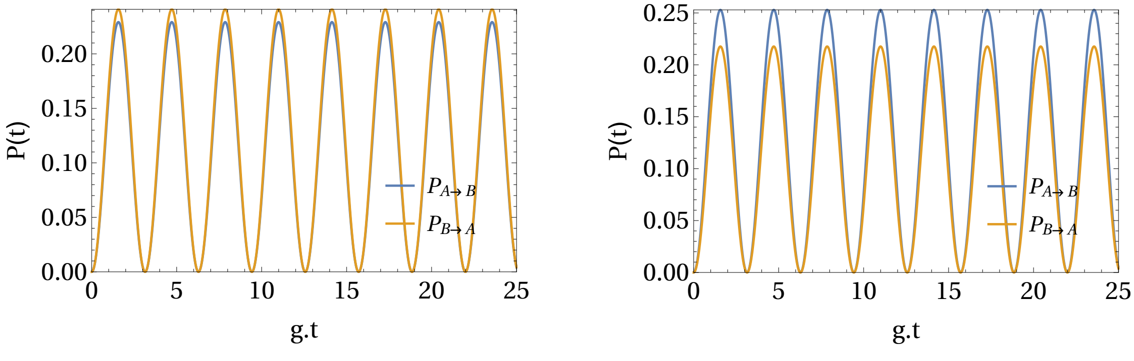
Using these results, the probability of A giving a particle for B and vice versa is

$$P_{A\to B}(t) = n_{A,k}(1 - n_{B,k})(1 - e^{-\lambda t} cos(2G_k t)) \tag{7.40}$$

and

$$P_{B\to A}(t) = n_{B,k}(1 - n_{A,k})(1 - e^{-\lambda t} cos(2G_k t)) \tag{7.41}$$

where $n_{A,B}$ are the initial thermal occupation. An example of the evolution of these probabilities is given in fig. 7.3 and fig. 7.3 .

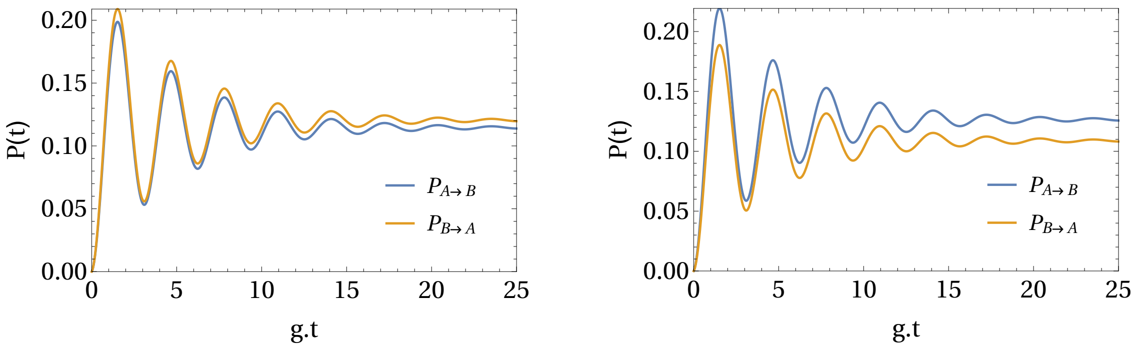


(a) $\delta\mu = 0$

(b) $\delta\mu = 0.2$

Figure 7.7: Systems prepared at $\lambda = 0$, $g = 1$, $T = 1\alpha$, $\mu = 1.5\alpha$, $\delta T = 0.1\alpha$, $k = \frac{2\pi}{3}$

In these graphics it is clear that the dephasing plays an important role in the termalization.



(a) $\delta\mu = 0$ (b) $\delta\mu = 0.2$

Figure 7.8: Systems prepared at $\lambda = 0.2$, $g = 1$, $T = 1\alpha$, $\mu = 1.5\alpha$, $\delta T = 0.1\alpha$, $k = \frac{2\pi}{3}$

For a unique momentum k, without dephasing the total system does not thermalize but for a non null dephasing, the systems will always thermalyze.

7.4 Fluctuation Theorem for the Bipartite System

7.4.1 Fluctuation Theorem for the Momentum k

In the previous section, we found the distributions of probabilities for a momemtum k, given by Eq.(7.40) and Eq.(7.41). Here, the variation of energy for a fixed momentum will be written as ϵ. Making the ratio between the probabilities, we obtain:

$$\frac{P_{A\to B}}{P_{B\to A}} = \frac{n_{A,k}(1-n_{B,k})}{n_{B,k}(1-n_{A,k})} = e^{(\epsilon_{A,k}-\mu_A)\beta_A} e^{-(\epsilon_{B,k}-\mu_B)\beta_B}. \tag{7.42}$$

Using

$$\Delta\epsilon_{A,k} = \epsilon_{A,k} = \epsilon_k, \qquad \Delta\epsilon_{B,k} = -\epsilon_{A,k} = -\epsilon_k \tag{7.43}$$

and

$$A_m = \beta_A\mu_A + \beta_B\mu_B, \qquad A_H = \beta_B - \beta_A \tag{7.44}$$

we obtain

$$\frac{P_{A\to B}([\Delta E_A, \Delta N_A]_k)}{P_{B\to A}(-[\Delta E_A, \Delta N_A]_k)} = e^{\Delta\epsilon_{A,k}A_H + \Delta N_{A,k}A_m} \tag{7.45}$$

with $\Delta E_{A,k} = -\epsilon$ and $\Delta N_{A,k} = -1$. So, this result agrees with the fluctuation theorem for energy and matter exchange, with the exchange of energy and particles expected with the assumptions.

7.4.2 Fluctuation theorem for the Full System

In this chapter it has already been shown that the resulting dynamics for a given momentum agrees with the fluctuation theorem for energy and matter exchange. However, for a lot of cases, the interest may be if the total process of the total system obeys the fluctuation theorem as well.

To work with the total system, we begin by remembering that different momentums are uncorrelated. Therefore, the probability of occuring two processes, each one for a determined momentum, is only the product of the probability of the two processes.

$$\frac{P_{A\to B}([\Delta E_A, \Delta N_A]_k + [\Delta E_A, \Delta N_A]_{k'})}{P_{B\to A}(-[\Delta E_A, \Delta N_A]_k - [\Delta E_A, \Delta N_A]_{k'})} = \frac{P_{A\to B}([\Delta E_A, \Delta N_A]_k)}{P_{B\to A}(-[\Delta E_A, \Delta N_A]_k)} \frac{P_{A\to B}([\Delta E_A, \Delta N_A]'_k)}{P_{B\to A}(-[\Delta E_A, \Delta N_A]'_k)}$$

$$\frac{P_{A\to B}([\Delta E_A, \Delta N_A]_k + [\Delta E_A, \Delta N_A]_{k'})}{P_{B\to A}(-[\Delta E_A, \Delta N_A]_k - [\Delta E_A, \Delta N_A]_{k'})} = e^{\Delta\epsilon_A A_H + \Delta N_A A_m} \tag{7.46}$$

Generalizing to the case of processes involving all modes of the system, we get:

$$\frac{P_{A\to B}([\Delta E_A, \Delta N_A]^{(i)})}{P_{B\to A}(-[\Delta E_A, \Delta N_A]^{(i)})} = \frac{\prod_k P_{A\to B}([\Delta E_A, \Delta N_A]_k)}{\prod_k P_{B\to A}([\Delta E_A, \Delta N_A]_k)} = \prod_k e^{\Delta\epsilon_{A,k} A_H + \Delta N_{A,k} A_m}. \tag{7.47}$$

Thereby, for many processes, the fluctuation theorem is

$$\frac{P([\Delta E_A, \Delta N_A]^{(i)})_{A\to B}}{P(-[\Delta E_A, \Delta N_A]^{(i)})_{B\to A}} = e^{\sum_k \Delta\epsilon_{A,k} A_H + \Delta N_{A,k} A_m}. \tag{7.48}$$

The upper indice (i) is just a label of a determined process.

7.5 Probability Distribution of Heat

In this section I will discuss the distribution of heat for some cases when $t \to \infty$ for chains with a number of sites N. For simplicity we set the chemical potential difference to zero, so that the flow of energy now coincides with the flow of heat. Moreover, the chemical potential in this analysis is fixed in $\mu = 0.4$. This value was chosen due to the fact that this value lies in an interval where we have a lot of possibilities of exchange of particles. In addition, I chose relatively high temperatures because they increase the occupations for higher energy levels, giving us the possibility of more combinations of exchange. The results are shown in Figs. (7.9-7.12). As a final remark, the histograms were based on 50.000 events each. This value was chosen due to the convergence in the behavior of the distribuition.

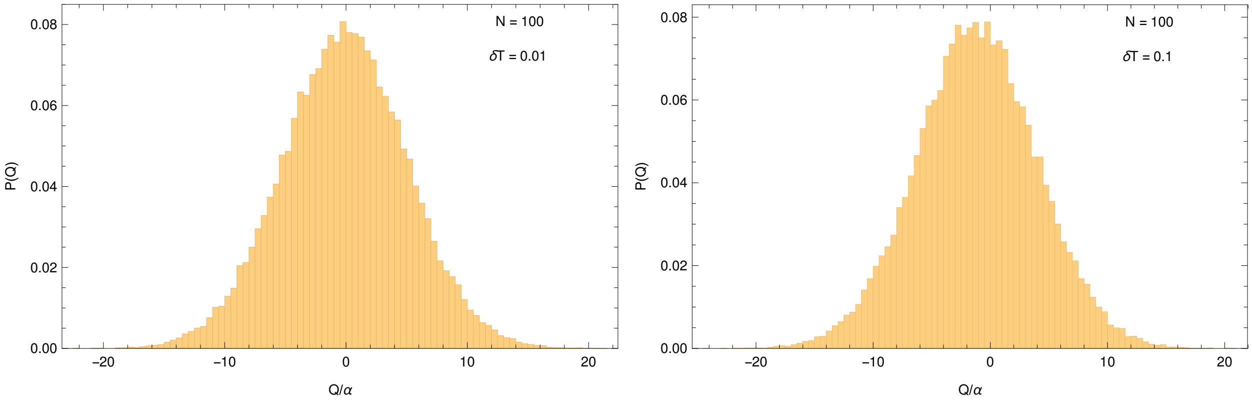


Figure 7.9: Probability distribution of heat for $N = 100$, $T = 1\alpha$ and different δn.

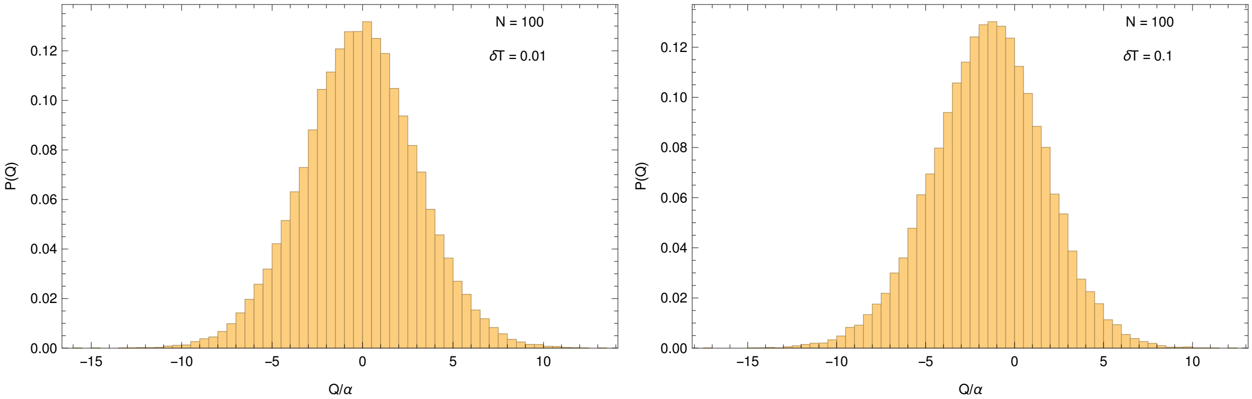


Figure 7.10: Probability distribution of heat for $N = 100$, $T = 0.5\alpha$ and different δn.

The increase of the occupation of higher energy levels when we increase the temperature is confirmed by comparing Fig.(7.9- 7.10) and Fig.(7.11- 7.12). As soon as we increase the temperature, the range of possible exchanged heats increases as well, indicating the raise of the probability for the high energy states to be occupied. This is another way to see the result given by

$$P_{A\to B}(t) = n_A(1-n_B)(1-e^{-\lambda t}cos(2G_k t)) \tag{7.49}$$

and

$$P_{B\to A}(t) = n_B(1-n_A)(1-e^{-\lambda t}cos(2G_k t)) \tag{7.50}$$

for $t \to \infty$. The advantage of this method is that we do not need to analyze the energy levels one by one, but instead, we can extract the same results by analyzing the exchanged heats.

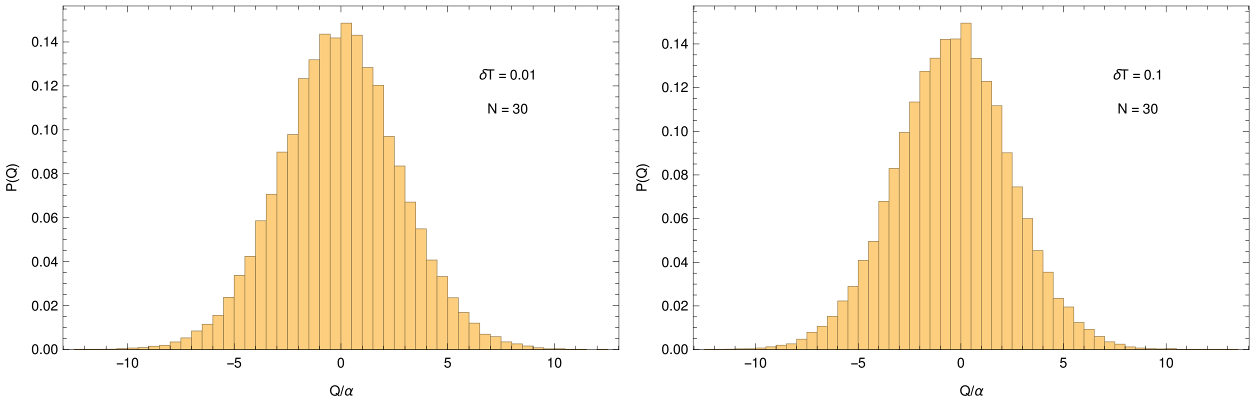


Figure 7.11: Probability distribution of heat for $N = 30$, $T = 1\alpha$ and different δn.

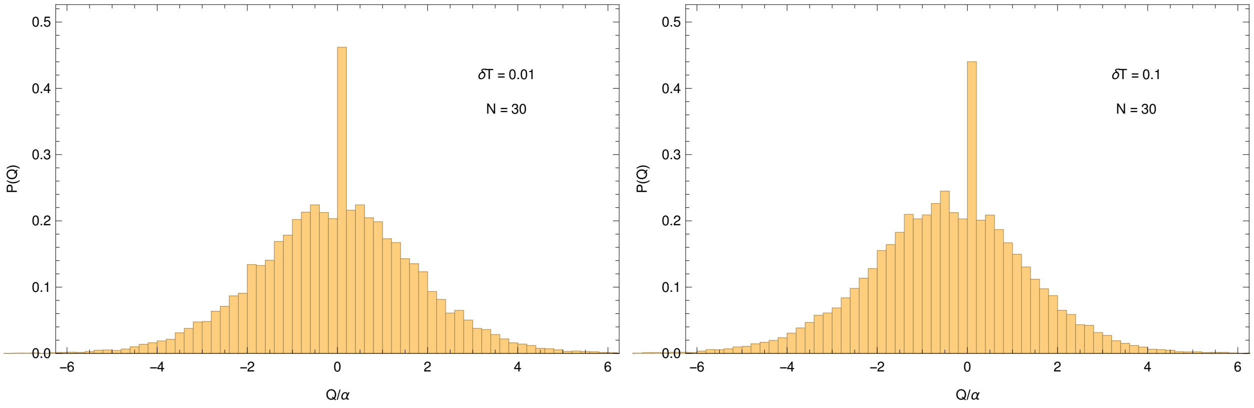


Figure 7.12: Probability distribution of heat for $N = 30$, $T = 0.5\alpha$ and different δn.

When we compare the figures with different numbers of sites, but with the other indentical conditions, we can note that the range of possible exchange of heat increases as soon as the number increases too. This fact can be easily explained just remembering that the number of states increases with the number of sites in a ratio one to one. It is clear that when we add possibilities of occupation, we do too for the possible heat exchanges. Comparing the figures with same temperature and number of sites but different δT, we see a deviation of the curve. It can be explained again just remembering that an increase of temperature increases the number of possible occupied states, making the exchange of particles and, as consequence, the exchange of heat possible.

Chapter 8

Conclusions and Final Remarks

In this dissertation we studied the out-of-equilibrium properties of quantum fermionic chains subject to gradients of temperature and chemical potentials.

The Hamiltonian of the system was written using the language of second-quantization and was considered that it obeys a tight-binding model. In order to diagonalize the Hamiltonian and find the eigen-energies of the system, we considered a weak coupling between the two halves. The weak coupling had a very important role in the analytical solutions because it allowed us to uncouple the modes with different k. Thanks to this, we were able to analyze the fluxes of particle and energy for each momentum separately as well as the mutual information and the evolution of the entropies. Finally, the uncoupling of the momentums allowed us to determine the validity of a fluctuation theorem for all states starting from fluctuation theorem applied to a given state of momentum k.

In order to study the influence of a dephasing in a system, the Lindblad master equation was used to compute the evolution of the density matrix and mean values. An evolution for a closed system is possible to obtain just by taking the coupling with the environment equal to zero. The dephasing was chosen in the basis of the Hamiltonian (previously diagonalized) having as assumption that the operator L used on the non-unitary part of the evolution had to be hermitian and it commutes with the Hamiltonian.

The dephasing noise had a very important role in the thermalization of the system. Its effects can be observed in the entropy production, the disappearance of the mutual information, and, consequently, the correlations, as time flows and obtaining the equilibrium for the total heat and number of particles exchanged more rapidly as it was possible to see in the previous chapter. An important remark is that, for systems prepared with small difference of occupations δk, we were able to find an analytical result for the study of each energy level.

Once we determined the evolution of the density matrix, we were able to compute explicitly the time evolution of some probabilities and with this in hand, the exchange fluctuation theorem was verified for a given energy level. As said before, with the uncoupling of the energy levels, it was possible to check that the whole system obeys an exchange fluctuation theorem too. Still talking about the probabilities, we analyzed the distribution of heat for different sizes of systems and different temperatures when the system had already thermalized. The distribution of heat then, can tell us the importance of the initial occupation in the statistics of the system.

Finally, although we did not use fluxes of particles and heat directly, instead we used the total heat or number of particles that flowed until the time t per site, it was shown that Onsager's reciprocity is obeyed. The final "fluxes", the dependence of the number of sites, and what the behaviors of the evolutions were, were analyzed with different initial thermal equilibrium. In these analysis we observed how the initial conditions influence the evolution and the amount of heat and particle trying to diferentiate the influence of different values of temperatures and chemical potential. Moreover, for low temperatures, we obtained analytical expressions for the fluxes using the Sommerfeld expansion. The validity of the approximation was studied for different chemical potentials, showing that low temperature is relative to the chemical potential and mainly with the energy scales. As a final remark, looking at the evolution of the averages of the Hamiltonian, the expected value for $t \to \infty$ agrees very well with the expected one from the classical thermodynamics.

Lastly, this work gave us bases for future treatment of more complex systems. So, I will list some topics that may be reference for future works:

- Determine the dephasing noise starting from the Hamiltonian of System + Reservoir.
- Study the thermalization for bosonic chains, in order to determine how much similar or different the system behaves with different statistics.
- Study new types of coupling between the chains, in order to determine the influence of

the structure in the thermalization.

- Apply these techniques for 2D and 3D systems such as graphene (and similar chemical compounds) and crystals.
- Study time-dependent dephasing noises and search for possible influences of momentum/energy dependence on dephasing.

Appendix A

Kraus Maps

First of all, let us consider the following definitions:

Linear Map A linear map, also called a linear transformation is a mapping, in other words, a generelization of functions, $V \to W$ between two modules (including vector spaces) that preserves the operations of sum and scalar multiplication.

Trace Class: It is a class of operators whose trace has to be conserved under change of basis.

Completely Positive: A completely positive map is such that it keeps the positivity of the eigenvalues.

Now recall that a density operator is a non-negative operator with unit trace.

Mathematically, a quantum operation is a linear map ϕ between spaces H and G such that: i)If S is a density operator, $Tr(\phi(S)) \leq 1$ ii) ϕ is completely positive for any natural number n, and any square matrix of size n whose entries are trace class operators

$$S = \begin{pmatrix} S_{11} & \cdots & S_{1n} \\ \vdots & \ddots & \vdots \\ S_{n1} & \cdots & S_{nn} \end{pmatrix} \tag{A.1}$$

and which is non-negative, then

$$\phi(S) = \begin{pmatrix} \phi(S_{11}) & \cdots & \phi(S_{1n}) \\ \vdots & \ddots & \vdots \\ \phi(S_{n1}) & \cdots & \phi(S_{nn}) \end{pmatrix} \tag{A.2}$$

Kraus Operators

Kraus' theorem characterizes maps that model quantum operators between density operators of quantum state.

Theorem Let H and G be Hilbert spaces of dimention n and m respectly, and ϕ be a quantum operator taking the density matrix acting on H to those acting on G.

Then there are matrices that will be called as Kraus Operators,

$$\{B_i\}_{1 \leq i \leq nm} \tag{A.3}$$

mapping G to H such that

$$\phi(\rho) = \sum_i B_i^\dagger \rho_0 B_i. \tag{A.4}$$

Moreover

$$\sum_i B_i^\dagger B_i \leq 1. \tag{A.5}$$

Unitary Equivalence

Kraus matrices are not unequily determined by quantum operation ϕ, in general. The following theorem states that all systems of Kraus matrices which represents the same quantum operation are related by a unitary transformation.

Theorem Let ϕ be (not necessarily trace preserving) a quantum operation in a finite Hilbert space H with two representing sequences $\{B_j\}_{j \leq n}$ and $\{C_i\}_{i \leq n}$. Then there is a unitary $(u_{ij})_{ij}$ such that

$$C_i = \sum_j u_{ij} B_j. \tag{A.6}$$

Appendix B

Covariance matrix

It is very common to have the need to solve a time evolution of an operator in quantum mechanics. The covariance matrix gives us the relations between creation and annihilation operators. The diagonal entries are the mean occupation values and the nondiagonal entries are the correlations between the states.

The covariance matrix Θ has elements $\Theta_{kl} \equiv \langle a_k^\dagger a_l \rangle$. Using the time evolution given by the equation 5.27, the elements $\Theta_{kl} \equiv \langle a_k^\dagger a_l \rangle$ are found by solving

$$\frac{d\Theta_{kl}}{dt} = i \, \langle [H, a_k^\dagger a_l] \rangle + \langle \tilde{D}(a_k^\dagger a_l) \rangle \tag{B.1}$$

In this appendix I will only solve for fermionic creation and annihilation operators and for bosons I will only summarize the commutation relations, which are useful for the calculus for this case.

The physical difference emerges from the Pauli's Exclusion Principle. Mathematically the difference is not so big, we only have a change commutation $\iff$ anticommutation relations. For bosons, we have commutators relations and for fermions we have anti-commutators relations as is written below.

- Bosons

$$[a_i, a_j] = 0, \qquad [a_i^\dagger, a_j] = \delta_{ij} \tag{B.2}$$

- Fermions

$$\{a_i, a_j\} = 0, \qquad \{a_i^\dagger, a_j\} = \delta_{ij} \tag{B.3}$$

B.1 Covariance Matrix for Fermions

Here we will deduce the general equation for the covariance matrix for fermions. Let us begin with the unitary part:

$$\begin{aligned}
[H, a_k^\dagger a_l] &= \sum_{i,j} = W a_i^\dagger a_j a_k^\dagger a_l - \sum_{i,j} W a_k^\dagger a_l a_i^\dagger a_j \\
&= \sum_{i,j} W a_i^\dagger (\delta_{ij} - a_k^\dagger a_j) a_l - \sum_{i,j} W a_k^\dagger (\delta_{il} - a_i^\dagger a_l) a_j^\dagger \\
&= \sum_i W_{ik} a_i^\dagger a_l - \sum_j W_{lj} a_k^\dagger a_j \\
&= \sum_i \Big(W_{ik} a_i^\dagger a_l - W_{il} a_k^\dagger a_i \Big),
\end{aligned} \tag{B.4}$$

thus

$$\begin{aligned}
\langle [H, a_k^\dagger a_l] \rangle &= \sum_i W_{ik} \Theta_{il} - W_{li} \Theta_{ki} \\
&= W_{ki}^T \Theta_{il} - \Theta_{ki} W_{il}^T \\
&= [W^T, \Theta]_{kl}
\end{aligned} \tag{B.5}$$

and finally

$$\langle [H, a_k^\dagger a_l] \rangle = [W^T, \Theta]_{kl}. \tag{B.6}$$

Now it is necessary to compute the non-unitary that is given by:

$$\langle \tilde{D}(a_k^\dagger a_l) \rangle = \lambda \sum_i \Big[a_i^\dagger a_i a_k^\dagger a_l a_i^\dagger a_i - \frac{1}{2} \{ (a_i^\dagger a_i)^2, a_k^\dagger a_l \} \Big]. \tag{B.7}$$

First, we look at the first term of the sum [1], which I will call as I:

$$\begin{aligned} I &= \sum_i a_i^\dagger a_i a_k^\dagger a_l a_i^\dagger a_i \\ &= \sum_i a_i^\dagger(\delta_{ik} - a_k^\dagger a_i)(\delta_{il} - a_i^\dagger a_l)a_i \\ &= \sum_i (\delta_{ik} a_i^\dagger - a_i^\dagger a_k^\dagger a_i)(\delta_{il} a_i - a_i^\dagger a_l a_i), \end{aligned} \tag{B.8}$$

and consequently,

$$I = \delta_{kl} a_k^\dagger a_l - a_k^\dagger a_i^\dagger a_l a_i. \tag{B.9}$$

Now we can look at the second term of the sum [2], which I will call II:

$$\begin{aligned} II &= \sum_i \left\{(a_i^\dagger a_i)^2, a_k^\dagger a_l\right\} \\ &= \sum_i a_i^\dagger a_i a_k^\dagger a_l + a_k^\dagger a_l a_i^\dagger a_i \\ &= \sum_i a_i^\dagger(\delta_{ik} - a_k^\dagger a_i)a_l + a_k^\dagger(\delta_{il} - a_i^\dagger a_l)a_i \\ &= 2a_k^\dagger a_l + 2a_k^\dagger a_i^\dagger a_l a_i. \end{aligned} \tag{B.10}$$

Taking the averages and putting all of the results together, we find:

$$\frac{d\Theta_{kl}}{dt} = i = [W^T, \Theta]_{kl} + \lambda(\delta_{kl} - 1)\Theta_{kl} \tag{B.11}$$

---

[1] Up to the constants.

[2] Once again, up to the constants.

Appendix C

Bessel Functions

In this appendix I will treat an especial function that was used in order to find an analytical solution for the evolution of the system when we start with small temperatures. The Bessel function is a very important one and there are a lot of possible discussions around them, therefore I will only discuss a little their principal characteristics and the uses.

C.1 Generator Function

Albeit usually one begins to work with Bessel functions in differential equations, here I will start from a two-variable function, usually known as *generator function* and then we will analyze the properties of the Bessel functions.

The generator function $g(x,t)$ is

$$g(x,t) = e^{(\frac{x}{2})(t-\frac{1}{t})} \tag{C.1}$$

and expanding it in Laurent series we get:

$$e^{(\frac{x}{2})(t-\frac{1}{t})} = \sum_{n=-\infty}^{\infty} J_n(x)t^n. \tag{C.2}$$

Explicitly

$$e^{(\frac{x}{2})(t-\frac{1}{t})} = \sum_{r=0}^{\infty} \frac{t^r}{r!}(\frac{x}{2})^r \sum_{s=0}^{\infty} (-1)^s \frac{x}{2}^s \frac{t^{-s}}{s!}. \tag{C.3}$$

For a given fixed n, such that $n = r - s$,

$$e^{(\frac{x}{2})(t-\frac{1}{t})} = \sum_{n=-\infty}^{\infty} \sum_{s=0}^{\infty} (\frac{x}{2})^{n+2s} \Big(\frac{t^n}{(n+s)!} \Big) (-1)^s, \tag{C.4}$$

and then

$$g(x,t) = \sum_{n=-\infty}^{\infty} \sum_{s=0}^{\infty} (\frac{x}{2})^{n+s} \Big(\frac{t^n}{(n+s)!} \Big) (-1)^s. \tag{C.5}$$

Comparing the equation Eq.C.1 and Eq.C.5, we find:

$$J_n(x) = \sum_{s=0}^{\infty} (\frac{x}{2})^{n+s} \Big(\frac{(-1)^s}{(n+s)!} \Big). \tag{C.6}$$

As it can be seen in Fig. C.1, the Bessel functions oscillate but they are not *periodic*, except when $x \to \infty$. In this case the amplitude falls asymptotically with $x^{-1/2}$.

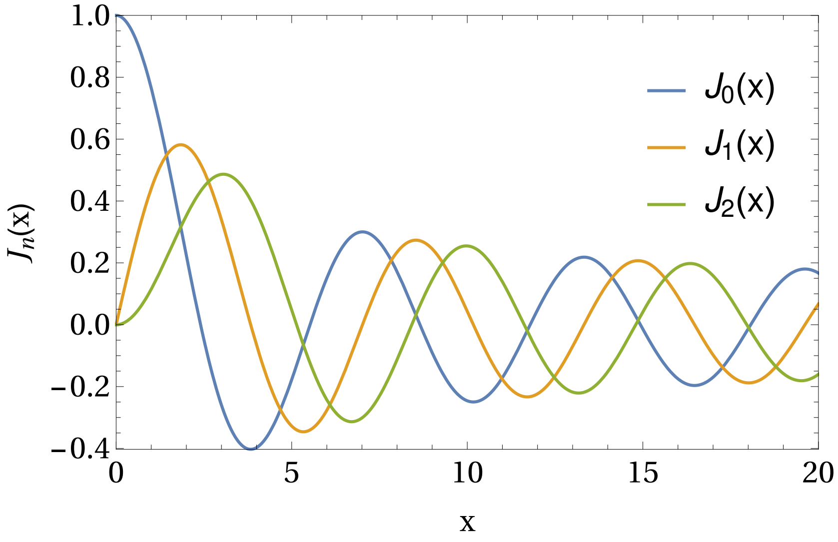


Figure C.1: Bessel functions for $n = 0, 1, 2$.

For $n < 0$ we get the following expression:

$$J_{-n}(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{s!(s-n)!} \Big(\frac{x}{2} \Big)^{2s+n}, \tag{C.7}$$

and consequently, one is able to see that

$$J_{-n}(x) = J_n(x). \tag{C.8}$$

C.2 Recurrence Relations

In this section we search for some recurrence relations. So, let us start with the generator function. Taking the derivative with respect to time, it is obtained:

$$\begin{aligned}
\frac{\partial g(x,t)}{\partial t} = \frac{x}{2}\left(1+\frac{1}{x^2}\right)e^{\left(\frac{x}{2}\right)\left(t-\frac{1}{t}\right)} &= \sum_{n=\infty}^{\infty} nJ_n(x)t^{n-1} \\
\frac{x}{2}e^{\left(\frac{x}{2}\right)\left(t-\frac{1}{t}\right)} + \frac{x}{2T^2}e^{\left(\frac{x}{2}\right)\left(t-\frac{1}{t}\right)} &= \sum_{n=-\infty}^{\infty} nJ_n(x)t^{n-1} \\
\frac{x}{2}\sum_{n=-\infty}^{\infty} J_n(x)t^n + \frac{x}{2}\sum_{n=-\infty}^{\infty} J_n(x)t^{n-2} &= \frac{x}{2}\sum_{n=-\infty}^{\infty} nJ_n(x)t^{n-1} \qquad \text{(C.9)}
\end{aligned}$$

Taking the terms with the same order in t, it is found

$$\frac{x}{2}(J_n(x) + J_{n-2}(x)) = nJ_{n-1}(x) \tag{C.10}$$

and therefore,

$$J_{n+1}(x) + J_{n-1}(x)) = \frac{2n}{x}J_n(x). \tag{C.11}$$

In order to find another recurrence relation, now we start differentiating the generator function with respect to x.

$$\begin{aligned}
\frac{\partial g(x,t)}{\partial t} = \frac{1}{2}\left(t-\frac{1}{t}\right)e^{\frac{x}{2}\left(t-\frac{1}{t}\right)} &= \sum_{n=-\infty}^{\infty} J_n'(x)t^n \\
\frac{1}{2}\sum_{n=-\infty}^{\infty} J_n(x)t^{n+1} - \frac{1}{2}\sum_{n=-\infty}^{\infty} J_n(x)t^{n-1} &= \sum_{n=-\infty}^{\infty} J_n'(x)t^n \qquad \text{(C.12)}
\end{aligned}$$

$$J_{n-1}(x) - J_{n+1}(x) = 2J_n'(x). \tag{C.13}$$

Combining Eq. C.11 and Eq.C.13 two more relations, can be seen below.

$$\frac{d}{dx}[x^n J_n(x)] = x^n J_{n-1}(x) \tag{C.14}$$

$$\frac{d}{dx}[x^{-n} J_n(x)] = -x^{-n} J_{n+1}(x) \tag{C.15}$$

C.3 Bessel's Differential Equation

Bessel's functions are naturally a solution of a kind of differential equation. Once we already know their properties, let us find the related differential equation. Using the equations Eq. (C.11) and Eq.(C.13) one more time we find

$$xJ'_n(x) = xJ_{n-1}(x) - nJ_n(x). \tag{C.16}$$

Taking the derivative with respect to x, it is obtained:

$$xJ''_n(x) + (n+1)J'_n(x) - xJ'_{n-1}(x) - J_{n-1}(x) = 0. \tag{C.17}$$

Using the recurrence relations in order to write this equation as dependence only of the n^{th} term, it is obtained:

$$x^2J''_n(x) + xJ'_n(x) + (x^2 - n^2)J_n(x) = 0. \tag{C.18}$$

It is clear then that $J_n(x)$ is the solution of a generic diffeerential equation

$$x^2y''(x) + xy'(x) + (x^2 - n^2)y(x) = 0. \tag{C.19}$$

C.4 Integral Picture

Something very useful in Bessel's function is its integral form. For this, first we take the generator function and use $t = e^{i\theta}$:

$$g(x,t) = e^{\frac{x}{2}(t-\frac{1}{t})} \quad \rightarrow \quad g(x,t) = e^{ix\sin(\theta)}. \tag{C.20}$$

Expanding, it is found

$$e^{ix\sin(\theta)} = J_0(x) + 2[J_2(x)\cos(2\theta) + J_4(x)\cos(4\theta) + ...] + 2i[J_1(x)\sin(\theta) + J_3(x)\cos(3\theta) + ...] \tag{C.21}$$

and comparing with the Euler's formula $e^{i\phi} = \cos(\phi) + i\sin(\phi)$, it is obtained:

$$\begin{aligned} \cos(x\sin(\theta)) &= J_0(x) + 2\sum_{n=1}^{\infty} J_{2n}(x)\cos(2n\theta) \\ \sin(x\sin(\theta)) &= 2\sum_{n=1}^{\infty} J_{2n-1}(x)\cos((2n-1)\theta). \end{aligned} \tag{C.22}$$

These results are very important in this dissertation because with a convenient choice of θ, the Onsager's coefficient was obtained.

Even though they are the most important result for this dissertation, we can go further and obtain some simple results for very difficult integrals. If we remember

$$\begin{aligned} \int_0^{\pi} \cos(n\theta)\cos(m\theta)d\theta &= \frac{\pi}{2}\delta_{nm} \\ \int_0^{\pi} \sin(n\theta)\sin(m\theta) \quad d\theta &= \frac{\pi}{2}\delta_{nm}, \end{aligned} \tag{C.23}$$

we will directly find

$$\frac{1}{\pi}\int_0^{\pi} \cos(x\sin(\theta))\cos(n\theta)d\theta = J_n(x) \tag{C.24}$$

if n is even and zero otherwise just using the Eq. (C.22). Notwithstanding, we obtain

$$\frac{1}{\pi}\int_0^{\pi} \sin(x\sin(\theta))\sin(n\theta)d\theta = J_n(x) \tag{C.25}$$

if n is odd and zero otherwise in the same way. Summing the last two results, we see that

$$J_n(x) = \frac{1}{\pi}\int_0^{\pi} \sin(x\sin(\theta))\sin(n\theta) + \cos(x\sin(\theta))\cos(n\theta)d\theta \tag{C.26}$$

and then

$$J_n(x) = \frac{1}{\pi}\int_0^{\pi} \cos(n\theta - x\sin(\theta))d\theta \tag{C.27}$$

for any n.

Appendix D

Analytical Solution for the "Fluxes" of Energy and Particles

In this chapter, I will show the complete analytical solution for the fluxes of particles and energy used in Sec.(6.2.4). These analytical solutions are valid in the context of $N \gg 1$ and low temperatures using Sommerfeld expansion, discussed in Sec.(3.4.4).

D.1 Analytical Solution for the Flux of Particles

First, I begin with the flux of particles per site for chain A, defined by:

$$\frac{\langle N_A \rangle_t - \langle N_A \rangle_0}{N} = \sum_k \frac{(n_{A,k} - n_{B,k})}{2} \Big(e^{-\lambda t} \cos(2G_k t) - 1\Big). \tag{D.1}$$

Using the considerations above, the sum will be converted into an integral, as follows:

$$\begin{aligned} \frac{\langle N_A \rangle_t - \langle N_A \rangle_0}{N} &= \frac{1}{2\pi} \int_0^{\pi} (n_{A,k} - n_{B,k})(e^{-\lambda t} \cos(2gt \sin^2 k) - 1) dk \\ &\equiv \bar{N}_A - \bar{N}_B, \end{aligned} \tag{D.2}$$

where $\bar{N}_X$ is defined by:

$$\bar{N}_X \equiv \frac{1}{2\pi} \int_0^{\pi} n_{X,k} (e^{-\lambda t} \cos(2gt \sin^2 k) - 1) dk \tag{D.3}$$

with $X = A, B$. The difficult part then is to compute $\bar{N}_X$ and here is the point where we use the Sommerfeld expansion. Thus we get: [1]

$$\bar{N}_X = \frac{1}{2\pi}\left\{ \int_{-2}^{\mu} \frac{(e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4})) - 1)}{\sqrt{4-\epsilon^2}} d\epsilon + \frac{\pi^2 T_X^2}{6}\frac{\partial}{\partial \epsilon}\left[\frac{e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4})) - 1}{\sqrt{4-\epsilon^2}}\right]_{\epsilon=\mu_X}\right\}. \quad \text{(D.4)}$$

The problem in computing $\bar{N}_X$, definitively, is not the derivative term that appears when we make the Sommerfeld expansion. Thus, let us forget for a minute the second term and pay attention to the integral. Let us call, for simplicity, I the integral in Eq.(D.16):

$$I = \int_{-2}^{\mu} \frac{(e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4})) - 1)}{\sqrt{4-\epsilon^2}} d\epsilon. \quad \text{(D.5)}$$

Going back to the k dependence, we find:

$$\begin{aligned} I &= \int_0^{\arccos(\frac{-\mu}{2})} e^{-\lambda t}\cos(gt(1-\cos 2k)) - 1 dk \\ & e^{-\lambda t}\int_0^{\arccos(\frac{-\mu}{2})} \cos(gt)\cos(gt\cos 2k) + \sin(gt)\sin(gt\cos 2k) dk - \arccos(\frac{-\mu}{2}). \end{aligned} \quad \text{(D.6)}$$

Now, we divide our problem again and define

$$I_1 = \int_0^{\arccos(\frac{-\mu}{2})} \cos(gt\cos 2k) dk \quad \text{(D.7)}$$

and

$$I_2 = \int_0^{\arccos(\frac{-\mu}{2})} \sin(gt\cos 2k) dk. \quad \text{(D.8)}$$

Then we remember some fundamental relations given by Bessel functions:

$$\begin{aligned} \cos(x\sin\theta) &= J_0(x) + 2\sum_{n=0}^{\infty} J_{2n}\cos(2n\theta) \\ \sin(x\sin\theta) &= 2\sum_{n=0}^{\infty} J_{2n}\sin((2n-1)\theta). \end{aligned}$$

---

[1] Please, note: In order to simplify the notation, a lot of times I will not use the subindice X, but it is important to have in mind that we will be treating with temperatures and chemical potential of the systems $X = A, B$.

Making $\theta = (2k + \frac{\pi}{2})$ as a convenient choice, we can replace the relations given by Eq.(D.9) and then we obtain:

$$
\begin{aligned}
I_1 &= \int_0^{\arccos(\frac{-\mu}{2})} \Big[J_0(gt) + 2\sum_{n=1}^{\infty} J_{2n}(gt)(-1)^n \cos(4nk)\Big] dk \\
&= J_0(gt)\arccos(\frac{-\mu}{2}) + 2\sum_{n=1}^{\infty}(-1)^n \mathcal{W}_{2n}(\mu, gt)
\end{aligned}
\tag{D.9}
$$

and

$$
\begin{aligned}
I_2 &= \int_0^{\arccos(\frac{-\mu}{2})} 2\sum_{n=1}^{\infty} J_{2n}(gt)(-1)^n \sin((2n-1)(2k+\frac{\pi}{2}))dk \\
&= -2\sum_{n=1}^{\infty}(-1)^n \mathcal{W}_{2n-1}(\mu, gt),
\end{aligned}
\tag{D.10}
$$

where I defined

$$
\mathcal{W}_n^{(1)}(\mu, gt) = \frac{J_n(gt)}{2n}\sin(2n\arccos(\frac{-\mu}{2})).
\tag{D.11}
$$

Putting all results together, we finally find:

$$
\begin{aligned}
\bar{N}_X &= \frac{1}{2\pi}\Bigg\{e^{-\lambda t}\Big[\cos(gt)\Big(J_0(gt)\arccos(\frac{-\mu}{2}) + \sum_{n=1}^{\infty}(-1)^n\mathcal{W}_{2n}(\mu, gt)\Big) + \sin(gt)\sum_{n=1}^{\infty}(-1)^n\mathcal{W}_{2n-1}(\mu, gt)\Big] \\
&+ \frac{\pi^2T^2\mu}{6}\Big[\frac{e^{-\lambda t}\cos(2gt(1-\frac{\mu^2}{4}))-1}{(4-\mu^2)^{3/2}} + \frac{2gte^{-\lambda t}\sin(2gt(1-\frac{\mu^2}{4}))}{\sqrt{4-\mu^2}}\Big] - \arccos(\frac{-\mu}{2})\Bigg\}.
\end{aligned}
\tag{D.12}
$$

The fluxes $J_{N,\mu}$ and $J_{N,T}$ are obtained directly by taking the derivatives of $\bar{N}_X$ with respect to μ and T, respectively.

D.2 Analytical Solution for the Flux of Energy

In the same way done for the flux of particles, we can obtain an analytical solution for the flux of energy. Then we start with:

$$
\frac{\langle H_A\rangle_t - \langle H_A\rangle_0}{N} = \sum_k \epsilon_k \frac{(n_{A,k}-n_{B,k})}{2}(e^{-\lambda t}\cos(2G_kt) - 1)\Big)
\tag{D.13}
$$

which can be converted into an integral in the thermodynamic limit.

$$\begin{aligned}\frac{\langle H_A\rangle_t - \langle H_A\rangle_0}{N} &= \frac{1}{2\pi}\int_0^{\pi} \epsilon_k (n_{A,k} - n_{B,k})(e^{-\lambda t}\cos(2gt\sin^2 k) - 1)dk \\ &\equiv \bar{E}_A - \bar{E}_B \end{aligned} \tag{D.14}$$

where we difine $\bar{E}_X$ as:

$$\bar{E}_X \equiv \frac{1}{2\pi}\int_0^{\pi} \epsilon_k n_{X,k}(e^{-\lambda t}\cos(2gt\sin^2 k) - 1)dk. \tag{D.15}$$

Using Sommerfeld expansion we get:

$$\bar{E}_X = \frac{1}{2\pi}\Bigg\{\int_{-2}^{\mu} \epsilon \frac{(e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4})) - 1)}{\sqrt{4-\epsilon^2}} d\epsilon + \frac{\pi^2 T_X^2}{6}\frac{\partial}{\partial \epsilon}\left[\epsilon_k \frac{e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4})) - 1}{\sqrt{4-\epsilon^2}}\right]_{\epsilon=\mu_X}\Bigg\}. \tag{D.16}$$

Once again, the derivative term is not the problem here. We will analyze the integral term separately.

$$\mathcal{I} = \int_{-2}^{\mu} \epsilon \frac{(e^{-\lambda t}\cos(2gt(\frac{4-\epsilon^2}{4})) - 1)}{\sqrt{4-\epsilon^2}} d\epsilon. \tag{D.17}$$

Going back to the k dependence we get:

$$\begin{aligned}\mathcal{I} &= \int_0^{\arccos(\frac{-\mu}{2})} -2\cos k(e^{-\lambda t}\cos(gt(1-\cos 2k)) - 1)dk \\ & e^{-\lambda t}\int_0^{\arccos(\frac{-\mu}{2})} -2\cos k(\cos(gt)\cos(gt\cos 2k) + \sin(gt)\sin(gt\cos 2k))dk + \sqrt{4-\mu^2}. \end{aligned} \tag{D.18}$$

Once again, we divide the problem into two, as follows:

$$\begin{aligned}\mathcal{I}_1 &= \int_0^{\arccos(\frac{-\mu}{2})} \Big[-2\cos k J_0(gt) + 2\sum_{n=1}^{\infty} J_{2n}(gt)(-1)^n(-2\cos k)\cos(4nk)\Big]dk \\ &= J_0(gt)\arccos(\frac{-\mu}{2}) + 2\sum_{n=1}^{\infty}(-1)^n \mathcal{W}_{2n}^{(2)}(\mu, gt) \end{aligned} \tag{D.19}$$

and

$$\begin{aligned}\mathcal{I}_2 &= \int_0^{\arccos(\frac{-\mu}{2})} 2\sum_{n=1}^{\infty} J_{2n}(gt)(-1)^n(-2\cos k)\sin((2n-1)(2k+\frac{\pi}{2}))dk \\ &= -2\sum_{n=1}^{\infty}(-1)^n\mathcal{W}^{(2)}_{2n-1}(\mu,gt), \end{aligned} \tag{D.20}$$

where I defined [2]

$$\mathcal{W}^{(2)}_n(\mu,gt) = J_n(gt)(\frac{\sin((2n+1)\arccos(\frac{-\mu}{2}))}{2n+1} + \frac{\sin((2n-1)\arccos(\frac{-\mu}{2}))}{2n-1}). \tag{D.21}$$

Putting all the results together, we finally obtain:

$$\begin{aligned}\bar{E}_X &= \frac{1}{2\pi}\Bigg\{\sqrt{4-\mu^2} + \frac{\pi^2T^2}{6}\Big[\frac{e^{-\lambda t}gt\mu\sin(2gt(1-\frac{\mu^2}{4})) + e^{-\lambda t}\cos(2gt(1-\frac{\mu^2}{4})) - 1}{\sqrt{4-\mu^2}} + \\ &+ \frac{\mu^2e^{-\lambda t}\cos(2gt(1-\frac{\mu^2}{4})) - \mu^2}{(4-\mu^2)^{3/2}}\Big] + e^{-\lambda t}\Bigg[\cos(gt)\Big(J_0(gt)\sqrt{4-\mu^2} + \\ &+ 2\sum_{n=1}^{\infty}(-1)^n\mathcal{W}^{(2)}_{2n}(\mu,gt)\Big]\Big) - \sin(gt)\Big(2\sum_{n=1}^{\infty}(-1)^n\mathcal{W}^{(2)}_{2n-1}(\mu,gt)\Big]\Big)\Bigg]\Bigg\}. \end{aligned} \tag{D.22}$$

D.3 Analysis of the Validity of the Analytical Solutions

In this section, I just show some pictures that was used to study the validity of the analytical solutions. We can see that the range in which the approximation is valid depends on the chemical potential, a feature yet observed on 3.4.4. Thus,it is shown for each case with its respective chemical potential, a value of temperature that the numerical and analytical results converges completely and one that they diverge lightly. This simple type of analysis gives us the interval of confidence for our analytical solution.

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[2] In the last step for $\mathcal{I}_1$ and $\mathcal{I}_2$, I used the exponential form of the cossines to make easier the obtaining of the results.

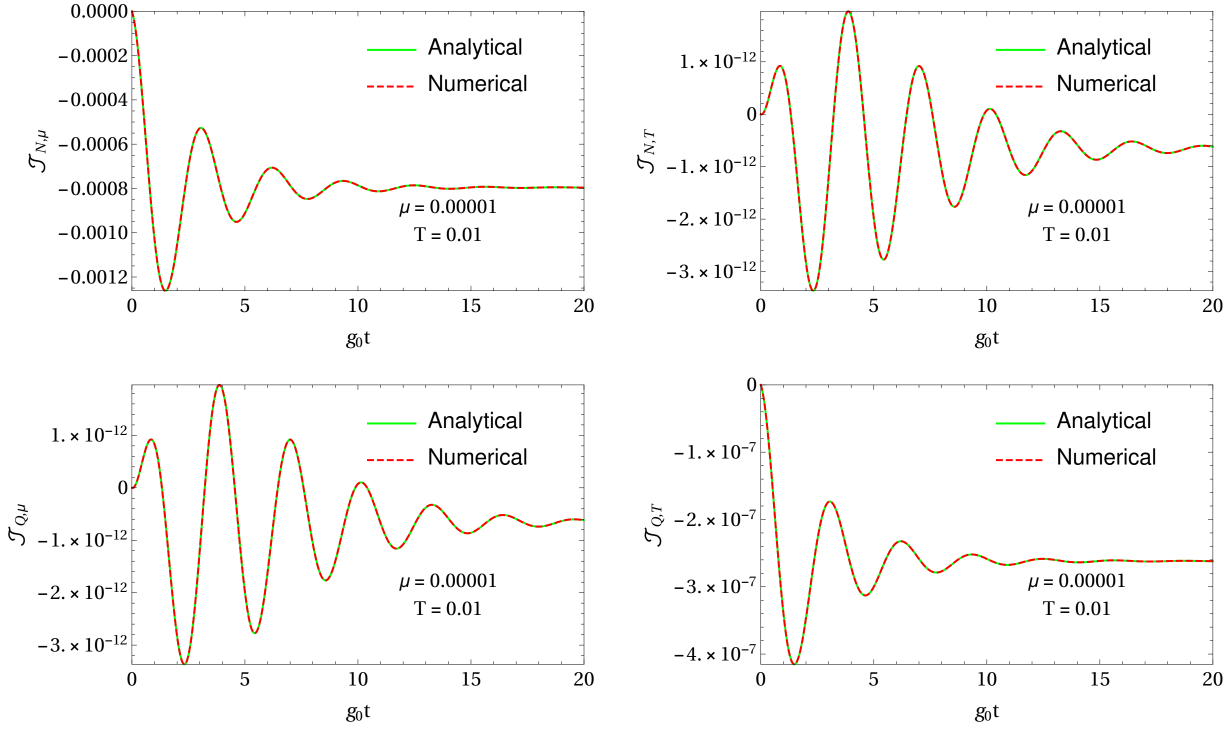

Figure D.1: Final exchanges.

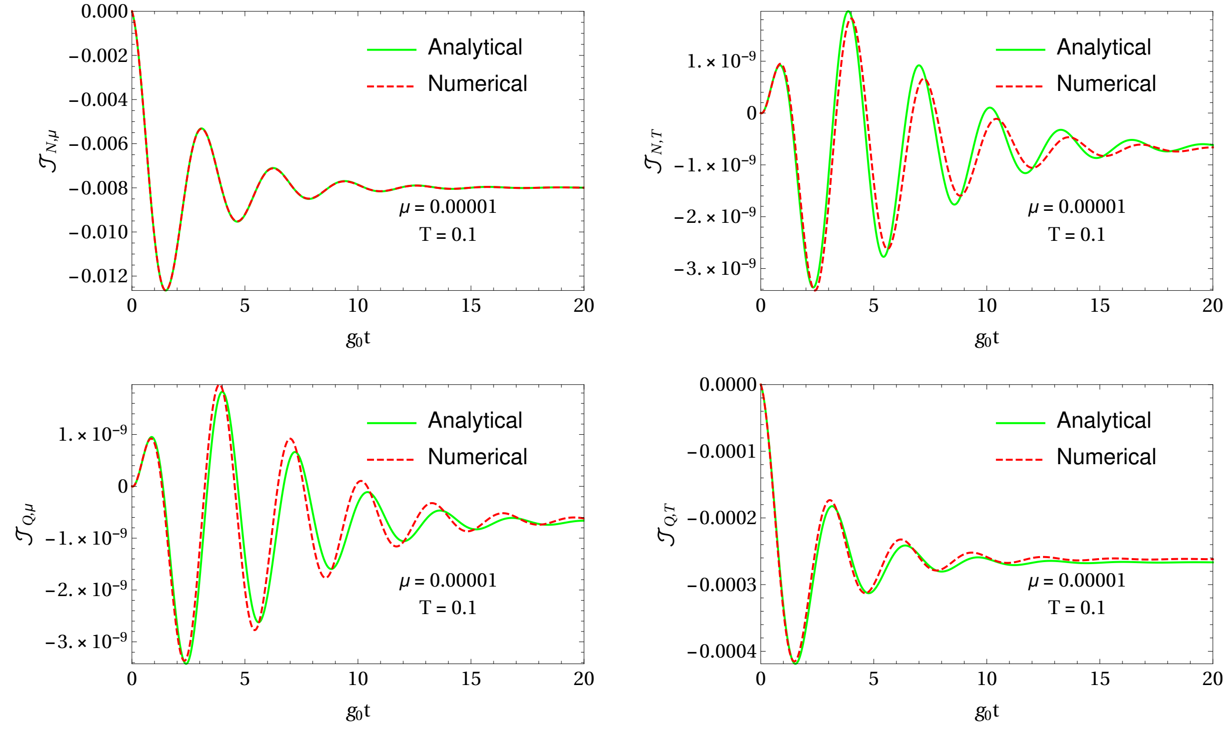

Figure D.2: Final exchanges.

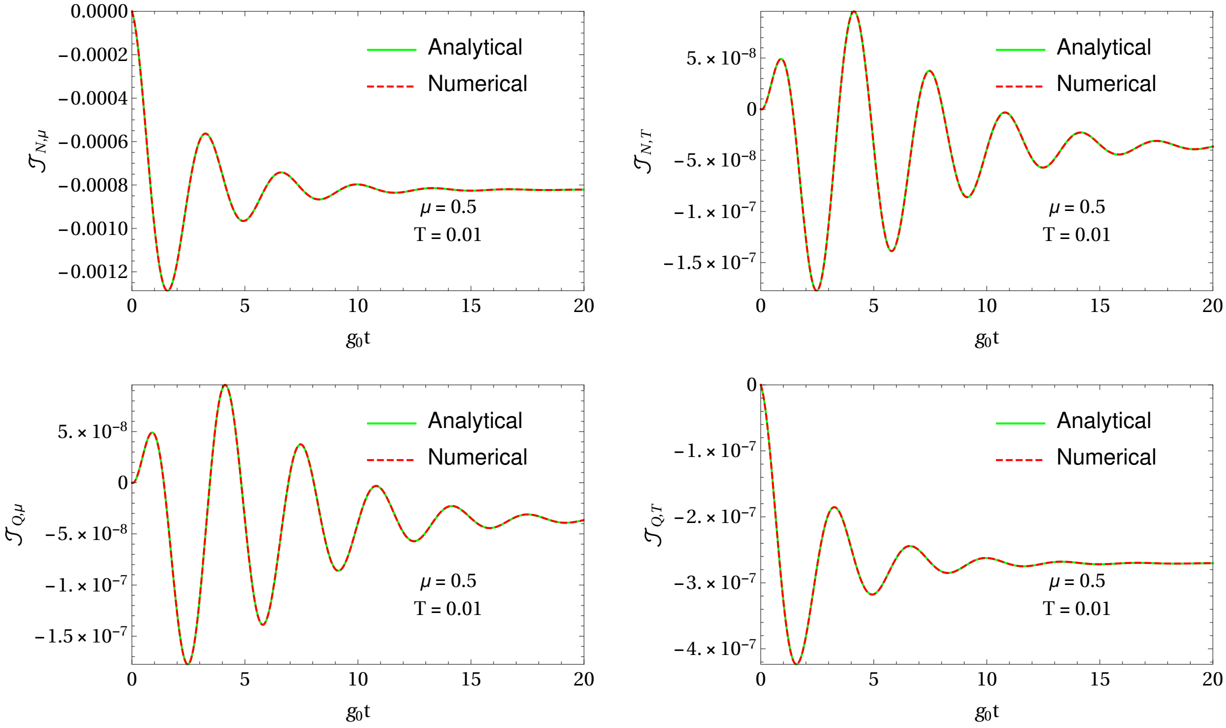

Figure D.3: Final exchanges.

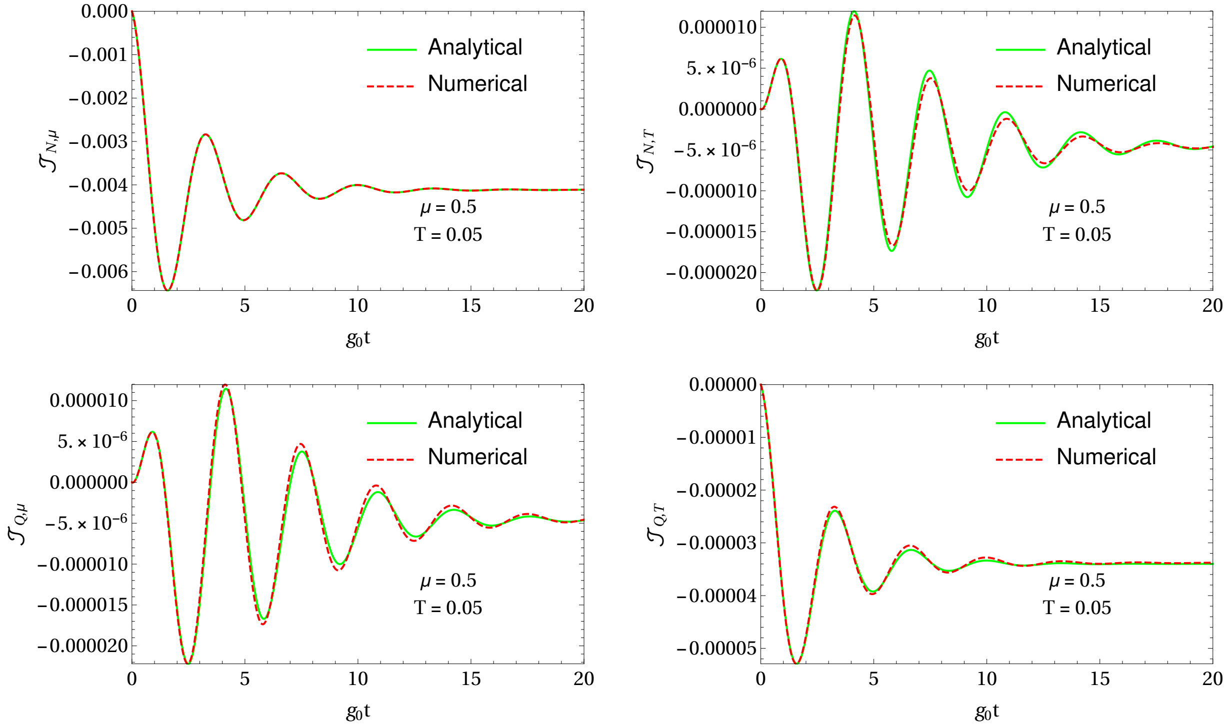

Figure D.4: Comparison between the analytical solution and the numerical solution.

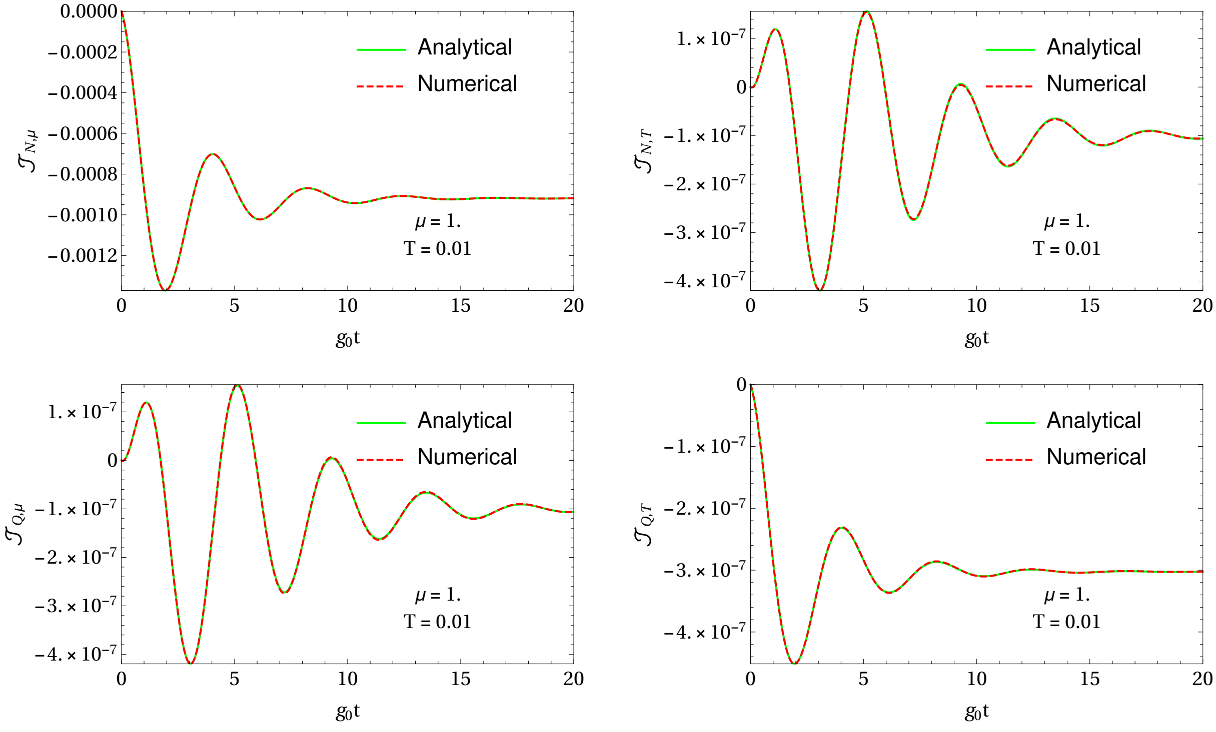

Figure D.5: Final exchanges.

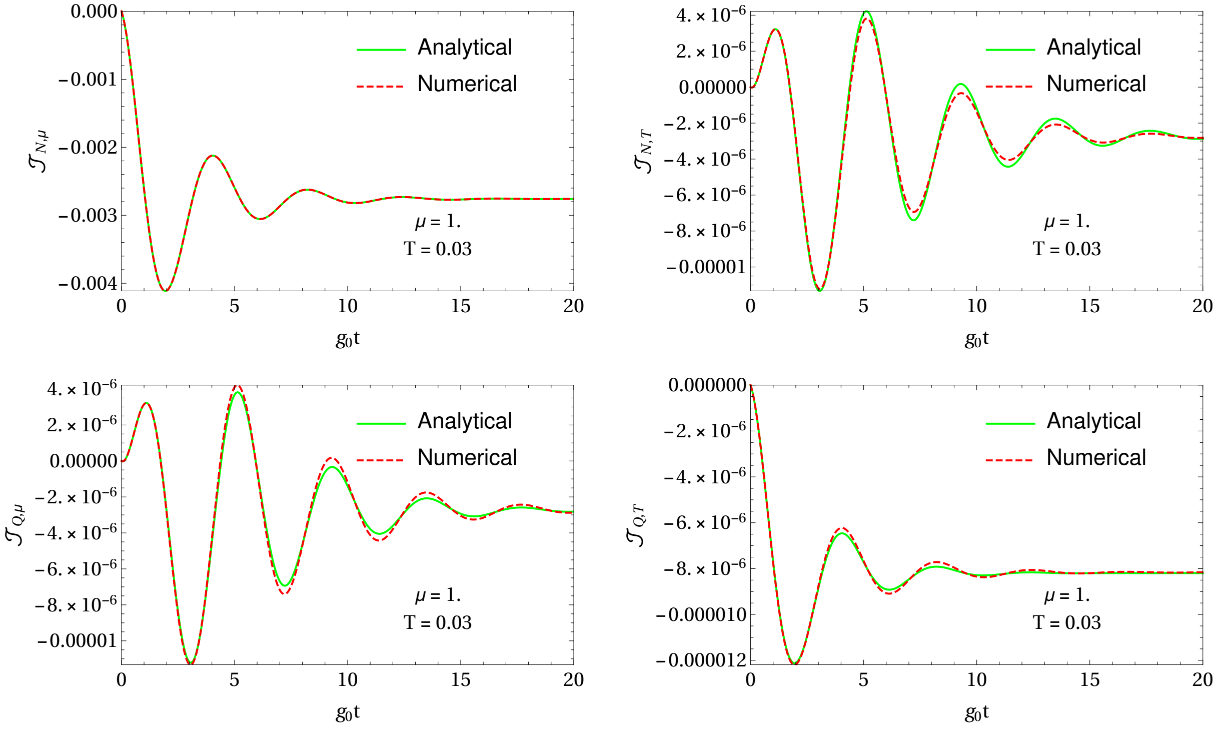

Figure D.6: Comparison between the analytical solution and the numerical solution.

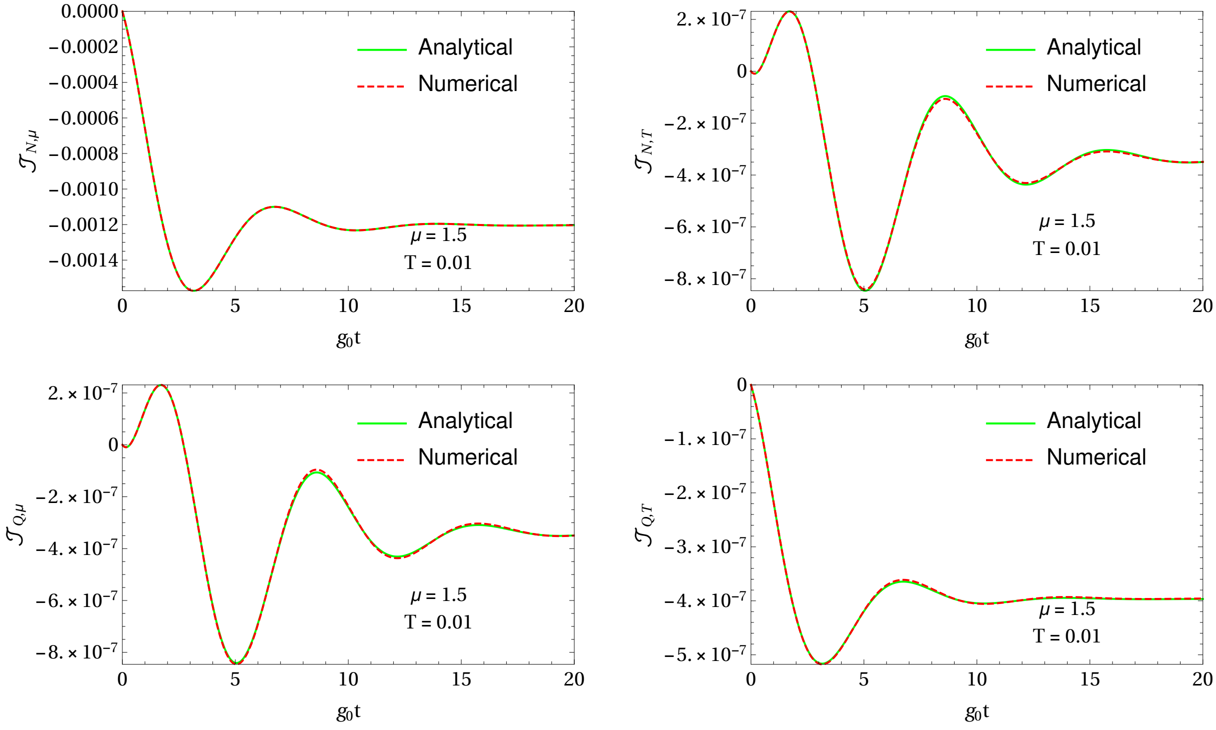

Figure D.7: Final exchanges.

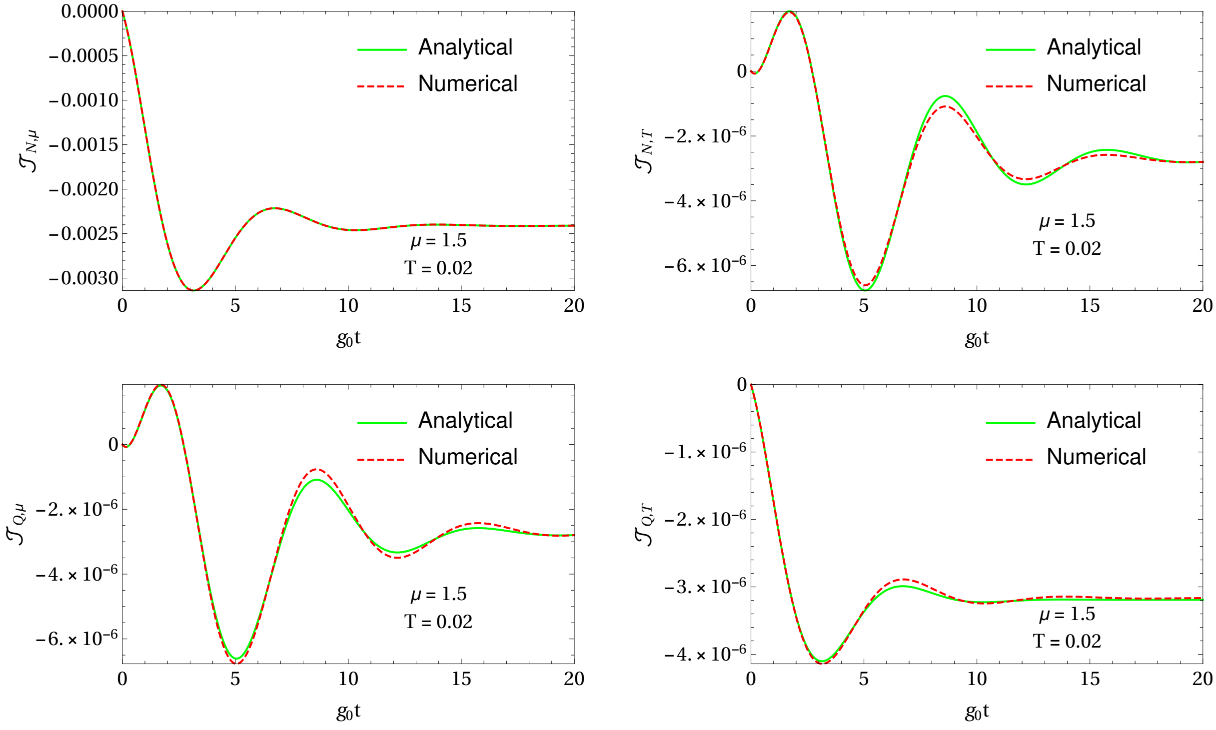

Figure D.8: Final exchanges.

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