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PT symmetric systems and thermodynamics

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Abstract

The present thesis will be mainly focused on two physical theories. First of all, we will discuss the non-Hermitian formulation of quantum mechanics, which is based on a class of Hamiltonians possessing a specific symmetry. Some topics to be discussed will be why they are physically acceptable and why we should be interested on them; additionally we will perform a simulation using a general quantum circuit.

On the other hand, the second part of the thesis will be focused on Thermodynamics. Specifically, we will be interested on how to measure the work performed on a quantum system by an external agent and how to simulate such thermodynamic process on a quantum computer.

We close the thesis with a discussion on how to merge these apparently unrelated fields in a single quantum circuit. In other words, we propose the path for simulating thermodynamic processes governed by non-Hermitian Hamiltonians in a quantum computer.

Contents

Chapter 1

Introduction

The developments brought by quantum mechanics and thermodynamics can hardly be quantified. From heat engines to quantum computers, these fields, which deeply changed our everyday life, lies in the basis of the present thesis.

Quantum mechanics establishes the laws of the microscopic world and rests in the core of modern technology, holding the promise to delivery a new revolution with the advent of quantum computers. Given a specific physical setup, the theory provides the probabilities of all possible measurements that can be performed on the system and how these probabilities evolve in time. The mathematical formalism is based on the introduction of Hermitian operators to represent physical quantities. This is natural since the eigenvalues of such operators, that represents the possible measurement outcomes, are real numbers. Among this class of operators, a very special one is the Hamiltonian $\boldsymbol{H}$, which is associated with the energy of the system and dictates how the state of the system evolves in time (and thus the probabilities). This symmetry ($\boldsymbol{H} = \boldsymbol{H}^\dagger$) implies that the time evolution operator $\boldsymbol{U} = e^{-i\frac{t}{\hbar}\boldsymbol{H}}$ is unitary, which is a necessary condition for the conservation of probabilities.

When dealing with open quantum systems, non-Hermitian Hamiltonians are employed to describe the effective dynamics of a system under dissipation. For instance, we can use an imaginary frequency in order to describe a damped harmonic oscillator. But, of course, this non-Hermitian Hamiltonian cannot be fundamental since it would imply a violation of unitarity of time evolution and, thus, probabilities would not be conserved.

However, in the past decades a new formulation of quantum mechanics emerged, based on the fact that, if a non-Hermitian Hamiltonian is invariant under the space and time reflections[1], then its spectrum is real and the unitarity of the time evolution is preserved [**?**]. A Hamiltonian with such a property is called $\mathcal{PT}$-symmetric. $\mathcal{P}$ stands for the space reflection operator, also known as parity operator, while $\mathcal{T}$ represents time reflection.

In this thesis we are interested in the simulation of $\mathcal{PT}$ symmetric systems in quantum computers. But these devices cannot directly implement non-Hermitian dynamics. However, it is possible to simulate a $\mathcal{PT}$ symmetric evolution by employing auxiliary quantum systems. The usual evolution operator, based on a Hermitian Hamiltonian, is applied to

[1] They also need to satisfy another condition that will be explained later.

the composed system (ancilla plus system of interest) and the ancillary system is measured at the end, resulting in an effective $\mathcal{PT}$ dynamics for the system of interest.

Regarding thermodynamics, it establishes emergent, statistical laws that systems with a huge number of degrees of freedom must obey[2]. In this limit, known as the thermodynamic limit, thermodynamics is based on three postulates. The one that is the most important here is the definition of the entropy function, that takes its maximum value for equilibrium states and cannot decrease in time. There are several ways to mathematically state this postulate, which is known as the second law of thermodynamics. The one that will be of particular relevance for the present thesis is that the work W done on a system —by some agent that performs a given process on it— is equal to the change in the free energy F, i.e. $W = \Delta F$. These quantities will be properly defined later on. This equation is valid for the case in which the working process is quasi-static, meaning that it is so slow that the system is in equilibrium all the time. When the process is performed in a finite amount of time, the system is taken out of equilibrium and entropy must be produced. In this case, the second law becomes an inequality $W \geq \Delta F$.

In the thermodynamic limit, fluctuations go to zero and the statistical nature of physical quantities like work and heat cannot be observed. What happens when we have a system with only a few degrees of freedom, like a molecule for instance? When fluctuations matter, new laws emerge. Such laws are known by the general name of fluctuation theorems and hold even for quantum systems [?]. Of course, in the quantum case, quantities like work and heat must be carefully defined. In such limit, physical quantities become random variables with an associated probability distributions. These probability distributions are defined when we consider infinitely many repetitions of the process. Although the second law of thermodynamics as stated above does not hold for systems out of the thermodynamic limit, we expect that this law is still valid on average, i.e. $\langle W \rangle \geq \Delta F$, where the average is taken over the probability distribution associated with the work. This is indeed the case.

By exploring interferometric ideas from quantum mechanics and quantum information theory, it was possible to experimentally investigate such relations, as will be discussed later. Actually, such ideas turn possible to simulate the out-of-equilibrium thermodynamics processes and to study the fluctuation relations for quantum systems in a quantum computer, a fact that lies in the core of the present thesis.

In the quantum case, fluctuation relations were studied considering that the Hamiltonian (usually time dependent) that characterizes the process under consideration is given by a Hermitian operator and only recently the case of $\mathcal{PT}$ symmetry was considered [?]. The main purpose of the present thesis is to consider the quantum simulation of the fluctuation relations for processes governed by $\mathcal{PT}$ symmetric Hamiltonians, thus merging both ideas discussed above. Specifically, we propose a quantum circuit whose output contains the information regarding the work probability distribution associated with a $\mathcal{PT}$ symmetric process.

The thesis is organized as follows. We start in Chapter 2 by describing the usual Hermitian quantum mechanics in order to set the notation and prepare the reader for the non-Hermitian case.

[2]Strictly speaking, we must take the thermodynamic limit, in which the number of degrees of freedom goes to infinity.

Chapter 3 briefly describes the $\mathcal{PT}$ symmetric formulation of quantum mechanics and the quantum circuit employed in order to simulate such systems in a quantum computer. We do not intend to provide a complete presentation of the theory here. Instead, we focus on the main aspects that will be used in the thesis and point the interested reader to references where the full theory is presented.
Changing subjects, Chapter 4 is devoted to the presentation of the Jarzynski equality for classical and quantum systems, which is one of the forms that the fluctuation theorems can take, while the quantum circuit developed for studying this relation in a quantum computer is discussed in Chapter 5.
Finally, Chapter 6 is devoted to our conclusions and the description of the quantum circuit for studying the fluctuation relations associated with a non-Hermitian, $\mathcal{PT}$ symmetric process.

Chapter 2

Hermitian Quantum mechanics

In this chapter we briefly describe the quantum formalism, focused on the reasons why the observables in such theory are postulated to be Hermitian, taking the Hamiltonian operator as the representative observable.

Quantum mechanics is based on a set of mathematical postulates. The first one states that the state of a quantum system is given by a vector in the Hilbert space. The second one is the dynamical equation governing the time evolution of this state, the Schrödinger equation. Finally, the third one connects the mathematical formalism with the physical world by stating that the quantum state should be viewed as an probability amplitude that determines, through Born's rule, the probabilities of the outcomes of all possible measurements that we can perform on the system.

When Quantum Mechanics was formulated back in 1920's, it was stated that the dynamics of a certain quantum system were governed by its Hamiltonian $\boldsymbol{H}$. The time evolution of the quantum state of a system is determined by the Schrödinger's equation

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

with $|\psi(t)\rangle$ being the quantum state of the system at time t.

The possible values that the energy of the system can take, E_a (which can be discrete), are given by the eigenvalues of the Hamiltonian and can be obtained by solving the associated eigenvalue equation

$$\boldsymbol{H}\left|\psi_a\right\rangle = E_a\left|\psi_a\right\rangle, \tag{2.1}$$

which is also known as the time-independent Schrödinger's equation. The set of vectors $\{|\psi_a\rangle\}$ defines the energy eigenbasis, on which the Hamiltonian takes a diagonal form. Given that the system is in state $|\psi(t)\rangle$, quantum mechanics tells us that the probability that an energy measurement will result in the outcome E_a is given by $p\left(E_a\right) = \left|\langle\psi_a|\psi_E\rangle\right|^2$.

From this discussion, it is clear that the engenvalues of the Hamiltonian (as well as of any other operator representing a physical quantity) must be real numbers. A way to assure this is by imposing that these operators, the observables, must be Hermitian ($\boldsymbol{H} = \boldsymbol{H}^\dagger$), where the symbol † stands for transposition and complex conjugation.

There is another reason why we should consider Hermitian operators and it is related with the conservation of probabilities. Schrödinger's equation determines that the quantum

state evolves accordingly with a unitary operator $\boldsymbol{U}$, such that $|\psi(t)\rangle = \boldsymbol{U}\,|\psi(0)\rangle$, with the time evolution operator satisfying the equation

$$\boldsymbol{H}\boldsymbol{U} = i\hbar\frac{\partial}{\partial t}\boldsymbol{U}.$$

In the simplest case in which the Hamiltonian does not depend on time, the solution of this equation is simply $\boldsymbol{U} = e^{-i\boldsymbol{H}t}$, which fullfils the unitarity condition $\boldsymbol{U}\boldsymbol{U}^\dagger = \boldsymbol{U}\boldsymbol{U}^{-1} = \mathbb{1}$ if the Hamiltonian is Hermitian, thus implying conservation of probability.

The reasons discussed above justify the postulate that observables should be represented by Hermitian operators.

Hermitian Hamiltonians have real eigenvalues and probabilities are conserved

The fact that a Hermitian operator has real eigenvalues is relatively easy to prove. As a matter of fact let us start with the eigenvalue equation (**??**). By projecting this equation on one of the energy eigenstates and then taking the conjugate transpose of the whole equation we obtain

$$\langle\psi_a|\,\boldsymbol{H}\,|\psi_a\rangle = E_a\,\langle\psi_a|\,\psi_a\rangle\,, \qquad \langle\psi_a|\,\boldsymbol{H}^\dagger\,|\psi_a\rangle = E_a^*\,\langle\psi_a|\,\psi_a\rangle\,. \tag{2.2}$$

Finally, we apply the condition for Hermiticity, i.e. $\boldsymbol{H} = \boldsymbol{H}^\dagger$, on the Hamiltonian in the conjugate equation (right). Then, equating the right-hand side of both equations we obtain $E_a = E_a^*$, from which we conclude that the eigenvalues of the Hamiltonian are real. Of course, this conclusion holds for any Hermitian operator.

Now, let us move to the conservation of probabilities under unitary dynamics. As it was stated in previous lines, the time evolution operator ($\boldsymbol{U} = e^{-i\frac{t}{\hbar}\boldsymbol{H}}$) resulting from a Hermitian Hamiltonian is ensured to be unitary.

Let us consider some normalized quantum state $|\psi\rangle$, which evolves in time via the time evolution operator, resulting the the state $|\psi'\rangle = \boldsymbol{U}\,|\psi\rangle$. Since the states are probability amplitudes, conservation of probability demands conservation of the norm of every state, which is guaranteed for unitary evolutions

$$\langle\psi'|\psi'\rangle = \langle\psi|\boldsymbol{U}^\dagger\boldsymbol{U}|\psi\rangle = \langle\psi|\psi\rangle = 1.$$

Notwithstanding the logic behind forcing the Hamiltonians to be Hermitian, these are not the only physically possible ones. Despite the fact that Hermitian operators have real spectra, the opposite statement does not hold in general. A real valued operator is not necessarily Hermitian. As we will see in the next chapter, there is a physically motivated symmetry that can be imposed on the system that keeps its eigenvalues real.

Therefore, imposing Hermiticity leaves many possible Hamiltonians out of reach. The reason for the physicists to be interested in those banned Hamiltonians is that they could be perfectly physical. What is more, they could make good models for many real physical systems. Therefore, it is our duty as physicists to explore the Hamiltonians beyond Hermiticity in order to discover whatever mysteries can be possibly hidden behind them.

Chapter 3

Non-Hermitian quantum mechanics on a quantum computer

The goal of this chapter is twofold. First, we introduce the non-Hermitian formulation of quantum mechanics based on Hamiltonian operators displaying a specific symmetry that ensures unitarity and the reality of the energy spectrum. Secondly, we discuss a quantum circuit that is able to simulate, in a quantum computer, any non-Hermitian evolution (within the presented theory).

Non-Hermitian quantum mechanics

Up to now, most undergraduate quantum physics students are taught that any quantum Hamiltonian needs to be Hermitian in order to be physical. This Hermiticity symmetry ensures that energy eigenvalues are real and time evolution is unitary. However, this requirement is not the only way to achieve these conditions, as we pointed out in the introduction.

In fact, developments made in the last decades [?, ?, ?] have shown that the Hermiticity condition may be replaced by another, more general, condition without giving up the physicality of the theory. A valid description of the physical system may be achieved imposing space-time reflection symmetry instead of the typical Hermiticity condition. Moreover, this new symmetry has the added benefit of being physically more transparent, comparing with the more mathematical Hermiticity requirement.

Let us now describe this symmetry, known as $\mathcal{PT}$ symmetry, in more details. It is composed by the space reflection operator (parity operator) $\mathcal{P}$ and the time reversal operator $\mathcal{T}$.

The effects of parity operator on the position and momentum operators are to reverse the sign of both of them

$$\mathcal{P}\boldsymbol{x}\mathcal{P} = -\boldsymbol{x} \qquad \mathcal{P}\boldsymbol{p}\mathcal{P} = -\boldsymbol{p},$$

while the action of the time reversal operator results in a change of sign of the momentum

$$\mathcal{T}\boldsymbol{x}\mathcal{T} = \boldsymbol{x} \qquad \mathcal{T}\boldsymbol{p}\mathcal{T} = -\boldsymbol{p}.$$

Nevertheless, time reversal operator also acts as the complex conjugation operation, by reversing the sign of the imaginary unity

$$\mathcal{T}i\mathcal{T} = -i.$$

This property implies that the time reversal operator $\mathcal{T}$ is not linear operator, but *antilinear* instead. Despite interesting, the special characteristics of this kind of operators will not be addressed in the present thesis.

Both $\mathcal{P}$ and $\mathcal{T}$ are reflection operators. Thus, if we apply them twice, it would be as if we made no changes at all. Mathematically

$$\mathcal{P}^2 = \mathcal{T}^2 = \mathbb{1}.$$

Additionally, $\mathcal{P}$ and $\mathcal{T}$ operators commute.

Once we described both $\mathcal{P}$ and $\mathcal{T}$ operators, we find ourselves in a position to define the $\mathcal{PT}$ symmetry. We define a $\mathcal{PT}$ reflected operator as

$$H^{\mathcal{PT}} \equiv (\mathcal{PT})H(\mathcal{PT}).$$

In this thesis we will consider Hamiltonians that are invariant under the action of this symmetry, which implies that the Hamiltonians should fulfill the condition

$$[\boldsymbol{H}, \mathcal{PT}] = 0.$$

This kind of Hamiltonian is called $\mathcal{PT}$ symmetric and has been proven to show unexpected properties. Since space-time reflection symmetry is weaker than Hermiticity one, a wider range of Hamiltonians may be accepted under the former, thus living us with entirely new ways to understand many phenomena in the world around us.

Nevertheless, the $\mathcal{PT}$ symmetric Hamiltonian is going to be a little trickier to work with (compared to the Hermitian one). In fact, as the $\mathcal{PT}$ operator is not linear, the eigenfunctions of a $\mathcal{PT}$ symmetric Hamiltonian may or may not be also eigenfuncitons of the $\mathcal{PT}$ operator. For this reason, it is of interest to us to define two situations for the symmetry: broken and unbroken.

When the eigenfunctions of the Hamiltonian do match with the ones of the $\mathcal{PT}$ operator the symmetry is called unbroken. In the case they do not match, then we will have a broken symmetry.

This particularity of the $\mathcal{PT}$ symmetric Hamiltonians is of great importance because it determines whether or not its eigenvalues are real. For those cases when the symmetry is unbroken, the eigenvalues will be real and the Hamiltonian will be physical. Otherwise, neither of those will happen. Proving this fact was not an easy task, but in the end it was done in 2001 [?,?,?] thanks to the discovery of the family of $\mathcal{PT}$ symmetric Hamiltonians in the form

$$\boldsymbol{H} = \boldsymbol{p}^2 + \boldsymbol{x}^2(i\boldsymbol{x})^k. \tag{3.1}$$

Where $k \in \mathbb{R}$. This is the most general form of a $\mathcal{PT}$ symmetric Hamiltonian, from which we can draw particular cases.

$\mathcal{PT}$ symmetric Hamiltonians have real eigenvalues when the symmetry is unbroken

In this section we will show what happens when we assume that $\mathcal{PT}$ and the Hamiltonian $\boldsymbol{H}$ share the same set of engenvectors. As mentioned above, due to the antilinear nature of the time reversal operator, this may not always be the case.

Let us begin with the eigenvalue equation for the $\mathcal{PT}$ operator

$$\mathcal{PT}\left|\psi_a\right\rangle = \lambda_a \left|\psi_a\right\rangle . \tag{3.2}$$

We can multiply this equation by $\mathcal{PT}$ from the left to obtain

$$(\mathcal{PT})^2 \left|\psi_a\right\rangle = (\mathcal{PT})\lambda_a \left|\psi_a\right\rangle . \tag{3.3}$$

Now, we make use of the fact $(\mathcal{PT})^2 = \mathbb{1}$ which implies

$$\left|\psi_a\right\rangle = \mathcal{PT}\lambda_a(\mathcal{PT})^2 \left|\psi_a\right\rangle , \tag{3.4}$$

thus resulting in

$$\left|\psi_a\right\rangle = \mathcal{PT}\lambda_a\mathcal{PT}\lambda_a \left|\psi\right\rangle \Rightarrow \left|\psi_a\right\rangle = \lambda_a^*\lambda_a \left|\psi_a\right\rangle , \tag{3.5}$$

where the complex conjugation is a consequence of the action of the time reversal operator. From this last equation we can clearly see that $|\lambda_a| = 1$, thus implying that $\lambda_a = e^{i\alpha_a}$ (for some set of real numbers α_a) is a pure phase.

Let us assume that the Hamiltonian shares the same set of engenvectors, i.e. $\boldsymbol{H}\left|\psi_a\right\rangle = E_a \left|\psi_a\right\rangle$. This implies that

$$\mathcal{PT}\boldsymbol{H}\left|\psi_a\right\rangle = \mathcal{PT}E_a(\mathcal{PT})^2 \left|\psi_a\right\rangle . \tag{3.6}$$

Additionally, as $\mathcal{PT}$ is antilinear, we know that $(\mathcal{PT})E(\mathcal{PT}) = E^*$. Therefore,

$$\boldsymbol{H}\lambda_a \left|\psi_a\right\rangle = E_a^*\lambda_a \left|\psi_a\right\rangle , \tag{3.7}$$

from which we obtain

$$E\lambda_a \left|\psi_a\right\rangle = E_a^*\lambda_a \left|\psi_a\right\rangle . \tag{3.8}$$

Consequently, as λ_a is non zero (equation (**??**)), the eigenvalues of the Hamiltonian must be real numbers, since we must have $E = E^*$.

As a general conclusion, we see that when $\boldsymbol{H}$ and $\mathcal{PT}$ operators shares the same set of engenvectors, the spectrum of $\boldsymbol{H}$ is real. This is the unbroken symmetry phase. Conversely, the $\mathcal{PT}$ symmetry is said to be broken when some of the eigenvectors of $\boldsymbol{H}$ are not simultaneously eigenvectors of the $\mathcal{PT}$.

Formalism

If we are to make use of this new kind of Hamiltonian, we will need to define a new formalism, which is going to be slightly different from the one used with Hermitian Hamiltonians. For our theory to be physical, we need it to fulfill the following requirements

- A well defined Hilbert space into which there is an inner product that implies a positive norm for all the vectors.
- The time evolution has to preserve the norm of the vectors, which implies it has to be unitary.

As a first approach, we can define the following inner product

$$(f, g) = \int [\mathcal{PT} f(x)] g(x) dx. \tag{3.9}$$

Considering this definition, if we compute the inner product between two eigenfunctions (ϕ_n and ϕ_m) of any $\mathcal{PT}$ symmetric Hamiltonian we will obtain the following result

$$(\phi_n, \phi_m) = (-1)^n \delta_{nm}. \tag{3.10}$$

This fact has been proven both analytically and numerically [**?**].

As it can be seem from equation (**??**), the norm associated with the $\mathcal{PT}$ symmetry is not positive definite. We cannot accept the fact that half of the energy eigenstates has a positive norm while the other half has a negative one. However, this fact may be caused by a symmetry owned only by the unbroken $\mathcal{PT}$ symmetric Hamiltonians, which we can be represented via the $\mathcal{C}$ operator

$$\mathcal{C}(x, y) = \sum_{n=0}^{\infty} \phi_n(x) \phi_n(y).$$

It is not difficult to see that the eigenvalues of $\mathcal{C}$ are

$$\mathcal{C}(x, y) \phi_n(x) = \sum_{m=0}^{\infty} \phi_m(x) \int \phi_m(y) \phi_n(y) dy = (-1)^n \phi_n(x),$$

where we have used Eq. (**??**) in the last step. From its eigenvalues, we can see how the freshly defined $\mathcal{C}$ operator represents a measurement of the $\mathcal{PT}$ norm (defined in equation (**??**)) of a certain eigenfunction of the $\mathcal{PT}$ symmetric Hamiltonian. Once these first definitions are set up, the inner product can be defined in terms of the $\mathcal{CPT}$ conjugation as

$$\langle \psi | \chi \rangle^{\mathcal{CPT}} = \int \psi^{\mathcal{CPT}}(x) \chi(x) dx,$$

where we defined $\psi^{\mathcal{CPT}}(x)$ as

$$\psi^{\mathcal{CPT}}(x) = \int \mathcal{C}(x, y) \psi^*(-y) dy.$$

With this definition of the inner product, the $\mathcal{C}$ operator would add an extra (-1) factor when acting on states with a negative $\mathcal{PT}$ norm[1]. Therefore, the inner product is now positive definite. In addition, the norm will be conserved in time[2] given that the Hamiltonian and the $\mathcal{CPT}$ operators commute with each other. Hence, as the two requirements we have stated earlier are met, $\mathcal{PT}$ symmetric Hamiltonians can be safely employed in order to formulate quantum mechanics.

[1] This is to say, for those cases where the $\mathcal{PT}$ inner product, defined in equation (**??**), is negative

[2] When the symmetry is unbroken, as was discussed earlier.

Example: Single qubit case

Now we have gotten a glance of the general non-Hermitian quantum mechanics, let us analyse a more specific case. It is going to be no other than the most simple qubit, the single one.

First of all, the general form of a Hamiltonian for a $\mathcal{PT}$ symmetric system can be written as

$$H_{\mathcal{PT}} = \begin{pmatrix} re^{i\theta} & s \\ \mu & re^{-i\theta}, \end{pmatrix} \tag{3.11}$$

for which we have an energy gap given by

$$\omega = 2\sqrt{\mu s - r^2 \sin^2\theta}.$$

Therefore, depending on whether the value of the gap is real or not we have an observable or not $\mathcal{PT}$ symmetry

$$\mu s - r^2 \sin^2\theta > 0 \Rightarrow \text{Symmetry observable},$$

$$\mu s - r^2 \sin^2\theta < 0 \Rightarrow \text{Symmetry not observable}.$$

As we already know, a $\mathcal{PT}$ symmetric Hamiltonian exhibits all the features of a quantum theory described by a Hermitian Hamiltonian, as long as the symmetry remains unbroken, otherwise it will not be a valid representation of the real world. Thus, in general, we will be interested in those parameter for which the symmetry is observable (unbroken). However, in the next sections we will analyse the differences between the observable and not observable cases. In particular, we shall compare how the system reacts in both situations.

Why are $\mathcal{PT}$ symmetric Hamiltonians interesting?

Up to now, we examined and described the $\mathcal{PT}$ symmetric Hamiltonians. However, apart from the fact that there are plenty of new Hamiltonians to choose from, there was no reason why should we be interested on them. This question is addressed here.

First of all, we will present the Brachistochrone problem and its relation with quantum mechanics.

Let us consider two dimensional surface, with an uniform gravity force acting downwards. Now we choose 2 (A and B) arbitrary points in the surface and draw an also arbitrary curve linking both points.

Given this situation, the statement of the brachistochrone problem would be: Which one is the curve that minimizes the time the ball takes to go from point A to point B? For the sake of simplicity, we will assume there is no friction between the ball and the ramp and that the intensity of the gravity does not change throughout the path of the ball.

An analogous problem could be defined in quantum mechanics. Let us imagine we have a system in an initial quantum state $|\psi_i\rangle$. Now, we would like it to go from that initial state

to another $|\psi_f\rangle$ one. How much time would it take? Which Hamiltonian would realize the transformation between those states in the least amount of time?

It is possible to prove that, for the case of Hermitian Hamiltonians, there exists a lower bound for the time the transformation is going to take [?]. However, it is also possible to round this limitation using $\mathcal{PT}$ symmetric Hamiltonians. This way, the aforementioned $|\psi_i\rangle \rightarrow |\psi_f\rangle$ transformation could be achieved in an arbitrarily low amount of time. Nevertheless, this accomplishment would take a certain Hamiltonian, one which may not be physically implementable.

Anyway, faster transitions between qubit states will always be an interesting goal to pursue. As a matter of fact, it would allow our quantum algorithms to run faster on a quantum computer.

Moreover, by looking at old phenomena from a different perspective may provide us a completely new approach to solve physical problems as well as new insights on the very basis of physics.

Simulating a $\mathcal{PT}$ symmetric Hamiltonian

In previous sections the theoretical aspects of the simulation were outlined. Now, in this section, we will present the actual simulation of a non Hermitian Hamiltonian as it is done in [?] and [?].

Duality Quantum Computing

As it was previously exposed, we are interested on simulating the evolution of a $\mathcal{PT}$ symmetric system. As it is not possible to directly perform such an evolution on a quantum computer, we will have to simulate it using auxiliary quantum systems, extra Qubits.

The approach we will take is explained in Refs. [?] and [?]. We describe here just the main aspects of the simulation, that will be useful for our later purposes.

The essence of the Duality Quantum Computing is to transform the initial state of the ancillary qubit into a linear superposition of many states [3]. Thereafter, the technique employs controlled quantum interference in order to map the information about the system of interest on the phase relations between the components of the supposition of the ancillary qubit state. We will illustrate how it works using the simplest possible implementation, where both system and ancilla are qubits, as shown in Figure **??**. From here on we consider the computational basis for the qubit, defined by the eigenstates of the Pauli operator σ_z, denoted by $|0\rangle$ and $|1\rangle$.

We will divide the circuit into 3 conceptual stages. The first Hadamard gate is the Quantum Wave Divider (QWD), the following V_1 and V_2 controlled gates will be the

[3] In our case, it will be divided into 2 states because we are working with qubits. However, it could also be divide into 3 in case we were using qutrits or, in general, the number of mutually orthogonal states our physical device allows us to use

Figure 3.1: Quantum circuit illustrating the Duality Computing. This is the simplest example of Duality and we use it for explanatory purposes. The upper qubit is the ancillary one while the bottom represents the system of interest. H is a Hadamard gate while V_1 and V_2 are given unitary operators acting on the system, controlled by the $|1\rangle$ and $|0\rangle$ ancillary qubit states, respectively.

unitary transformations we will need apply on each of the divided waves. Finally, the last Hadamard gate will be the Quantum Wave Combiner (QWC).

QWD's function is to create the initial superposition given the initial ancillary state $|0\rangle_a$. So, its action on the initial state $|\psi_d\rangle = |0\rangle_a |\psi_e\rangle$ is given by

$$|\psi_d\rangle = \frac{|0\rangle_a + |1\rangle_a}{\sqrt{2}} |\psi_e\rangle .$$

In the second stage, we have 2 controlled gates, each of which affect the second qubit only for a certain state of the ancillary qubit (V_1 $|0\rangle_a$-controlled while V_2 is controlled by $|1\rangle_a$). Therefore, after this stage, the state of the entire system is

$$|\psi_s\rangle = \frac{1}{\sqrt{2}} |0\rangle_a \boldsymbol{V_1} |\psi_e\rangle + \frac{1}{\sqrt{2}} |1\rangle_a \boldsymbol{V_2} |\psi_e\rangle .$$

Now it is time to combine the waves and look for the resulting interference pattern. This is done by the final Hadamard gate (QWC). The result is

$$|\psi_f\rangle = \frac{1}{2} |0\rangle_a (\boldsymbol{V_1} + \boldsymbol{V_2}) |\psi_e\rangle + \frac{1}{2} |1\rangle_a (\boldsymbol{V_1} - \boldsymbol{V_2}) |\psi_e\rangle .$$

Finally, if we measure the ancillary qubit and find it in the $|0\rangle_a$ state, then the second qubit would have evolved under the $\boldsymbol{V_1} + \boldsymbol{V_2}$ transformation, which is not necessarily unitary. This fact will be of great interest to us because our goal is to simulate a $\mathcal{PT}$ symmetric (thus, not always unitary) evolution. Therefore, if we achieve to write our evolution operator $e^{-i\boldsymbol{H}t}$ as $\boldsymbol{V_1} + \boldsymbol{V_2}$ we will be able to perform our desired simulation. One important point here is that an arbitrary $\mathcal{PT}$ symmetric Hamiltonian leads to a non-unitary evolution, in general. However, in order to acquire a physical meaning we need to look only for the unbroken phase. But the quantum circuit is able to simulate even a non physical Hamiltonian.

A general two qubit quantum circuit

Figure **??** shows a general quantum system that is able to simulate an arbitrary non-Hermitian Hamiltonian [**?**]. For the present case, we are keen on making the second Qubit be in the state $e^{-i\boldsymbol{H}t} |0\rangle$ when the first Qubit is in the $|0\rangle$ state.

By following the same procedure outline in the last section we obtain the following state at the output of the system

$$|\psi_f\rangle = \frac{1}{\sqrt{2}} |0\rangle_a (\cos\phi_V \boldsymbol{V_1} |0\rangle_e + \sin\phi_v \boldsymbol{V_2} |1\rangle_e) + \frac{1}{\sqrt{2}} |1\rangle_a (\cos\phi_V \boldsymbol{V_1} |0\rangle_e - \sin\phi_v \boldsymbol{V_2} |1\rangle_e) .$$

$$\begin{array}{llllll} |0\rangle & \mathrm{V} & 1 & 1 & \mathrm{H} \\ |0\rangle & \mathrm{R}_y(2\theta) & V_1 & V_2 & \end{array}$$

Figure 3.2: Quantum circuit that simulates a general $\mathcal{PT}$ symmetric system. It is achieved into the second qubit when the first one collapses into $|0\rangle$. $R_y(2\theta)$ is a rotation about y direction by the angle 2θ, while the other operators are defined in the text.

After projecting the ancillary qubit in the state $|0\rangle_a$, we obtain the final state of the system in the form

$$|\psi_f\rangle_e = \cos\phi_V \boldsymbol{V_1} |0\rangle_e + \sin\phi_v \boldsymbol{V_2} |1\rangle_e$$

Now, in order to simulate the evolution accordingly with the general Hamiltonian given in Eq. **??** we need to consider the following forms for the operators contained in the quantum circuit shown in figure **??**, which were derived in Ref. [**?**]

$$\begin{aligned} V &= \begin{pmatrix} \cos\phi_v & -\sin\phi_v \\ \sin\phi_v & \cos\phi_v \end{pmatrix}, \quad V_1 = \begin{pmatrix} \cos\phi_{v1} & i\sin\phi_{v1} \\ i\sin\phi_{v1} & \cos\phi_{v1} \end{pmatrix} \\ &\text{and} \quad V_2 = \begin{pmatrix} \cos\phi_{v2} & -i\sin\phi_{v2} \\ i\sin\phi_{v2} & -\cos\phi_{v2} \end{pmatrix}. \end{aligned} \tag{3.12}$$

The angles in this last equation are given by

$$\begin{aligned} \phi_v &= \arccos\left[\sqrt{\frac{\omega^2\cos^2(\frac{\omega t}{2\hbar}) + (\mu+s)^2\sin^2\left(\frac{\omega t}{2\hbar}\right)}{\omega^2\cos\left(\frac{\omega t}{\hbar}\right) + 2(\mu+s)^2\sin^2\left(\frac{\omega t}{2\hbar}\right)}}\right] \\ \phi_{v1} &= \arccos\left[\frac{\omega\cos\left(\frac{\omega t}{2\hbar}\right)}{\sqrt{\omega^2\cos\left(\frac{\omega t}{\hbar}\right) + (\mu+s)^2\sin^2\left(\frac{\omega t}{2\hbar}\right)}}\right] \\ \phi_{v2} &= \arccos\left[\frac{2r\sin\theta}{\sqrt{(\mu-s)^2 + 4r^2\sin^2\theta}}\right]. \end{aligned} \tag{3.13}$$

Figure **??** shows numerical simulations of the quantum circuit given in Fig. **??** for several values of θ. We found a very good agreement with the results reported in Ref. [**?**], thus confirming the validity of our simulations. Indeed, it is possible to prove that, when the state of the ancillary system is detected in $|0\rangle_a$, the state of the system at the output of the system is given by

$$|\psi(t)\rangle_e = e^{-i\boldsymbol{H}t} |\psi(0)\rangle_e, \tag{3.14}$$

with $|\psi(0)\rangle_e$ being the initial state of the system.

Entanglement restoration

Although we will not use entanglement for our proposal, in this section we study an extend circuit in which the system of interest in composed by two qubits and analyse the entanglement between then. This is useful in order to validate even further our numerical simulations.

As a proof of principle, we will simulate the entanglement restoration phenomenon for both unbroken and broken symmetry cases [**?**]. The circuit shown in Fig. **??** will be used for this

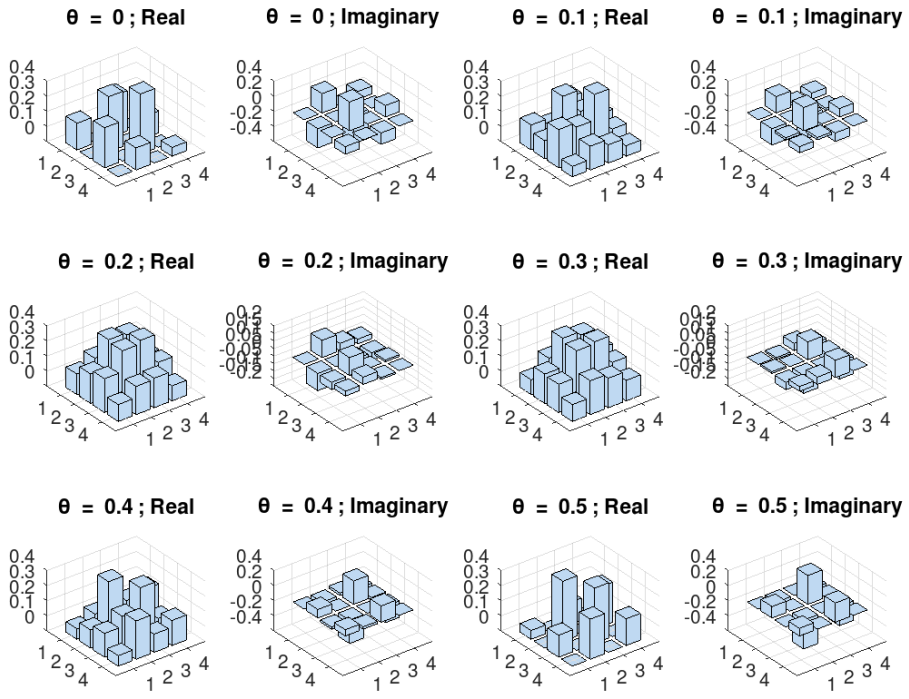

Figure 3.3: Results obtained from the simulation of the quantum circuit shown in Figure **??**. The θ value was varied from 0 to 0.5 π and the real and imaginary parts of the density matrix of the final state were plotted in this figure.

$$
\begin{array}{ccccccccc}
|0\rangle & [2]\mathrm{V} & 1 & 1 & 1 & 1 & \mathrm{H} \\
 & |0\rangle & 1 & 1 & 1 & 1 & \mathrm{H} \\
|0\rangle & \mathrm{H} & 1 & \mathrm{I} & \mathrm{X} & \mathrm{Y} & \mathrm{Z} \\
 & |0\rangle
\end{array}
$$

Figure 3.4: Quantum circuit implementing the entanglement restoration phenomenon. Analogously to the circuits discussed in the last section, we will focus on the state of the last two qubits when the first two are found in the state $|00\rangle$.

purpose. As can be seen in Fig. **??**, when the symmetry is unbroken (observable) then the entanglement restoration phenomenon occurs. Otherwise it does not, as it was expected. This figure shows the concurrence between the two qubits composing the system, which is a well known entanglement measure [**?**].

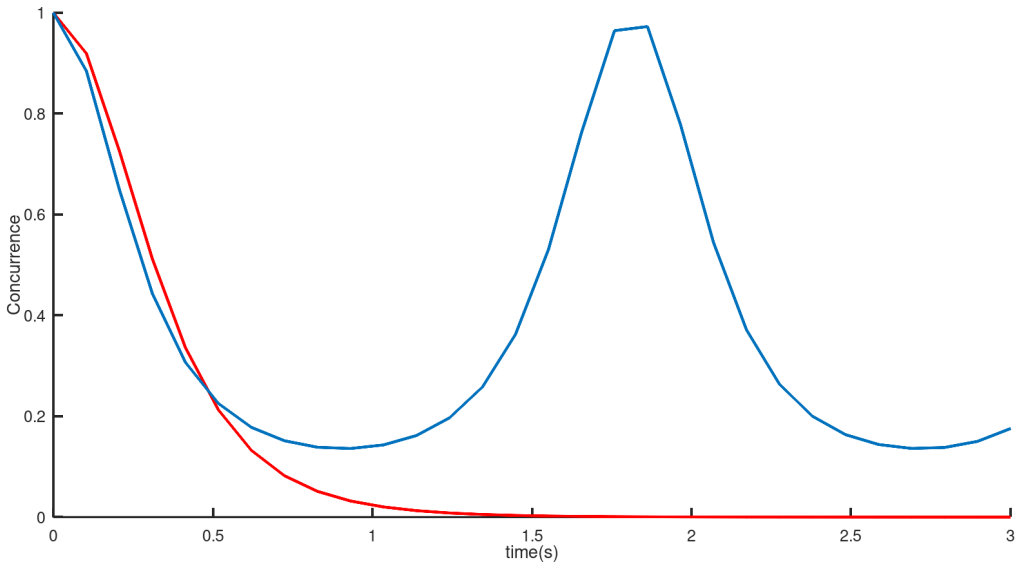

Figure 3.5: Relation between the concurrence of the last 2 qubits in **??**. The broken symmetry is shown in red, while the observable one is in blue. The entanglement restoration of the entanglement can be seen around $t = 2$, for the observable case.

Chapter 4

Jarzynski fluctuation relation

The present chapter of the thesis will be devoted to acquanint the reader with the Jarzynksi fluctuation relation, which is to be used later in the next chapter.

In 1997, C. Jarzinsky proved an exact relation between nonequilibrium quantities and equilibrium free energies [**?**]. To better explain this, let us consider a system in thermodynamical equilibrium sates A; now, a agent performs work on the system, taking it from state A to state B. In this situation, the performed work will be equal to the difference on the Helmholtz free energies of both states

$$W = F_B - F_A, \tag{4.1}$$

where $F_X = -\beta^{-1} \ln Z_X$, with β being the inverse temperature of the system and Z_X is the partition function of state X. This is one of the statements of the second law of thermodynamics and is valid only when the process is performed on a quasistatic manner. Otherwise the work is going to be bigger than the difference between the free energies of both states

$$W \geq F_B - F_A.$$

It is precisely this excess of work what is responsible for the generation of entropy. Indeed, the entropy produced by the process is given by $\Sigma = W - (F_B - F_A)$.

These results apply for the so called thermodynamic limit, where fluctuations vanish. Jarzynski considered a general system our of this limit, where fluctuations matter and proved that, for a classical systems under an arbitrary Hamiltonian process, the flollowing relation holds

$$\left\langle e^{-\beta W} \right\rangle = e^{-\beta(F_B - F_A)}. \tag{4.2}$$

In this relation, the average is taken over many repetitions of the process. This is much stronger than the second law of thermodynamics, which it implies. Equation (**??**) has deep implications, the most notable of them being that it links nonequilibrium (W) and equilibrium quantities (F_X). Therefore, it would make possible to acquire knowledge about the equilibrium state of the system without having direct access to the mentioned equilibrium state.

This can be illustrated with a simple example. Let us consider a chair in the macroscopic world. From our point of view, it has a definite position, temperature, volume, etc... However, if we look more closely, we will see the atoms of that same chair. Those atoms

will not have fixed position, temperature, or many other properties that seemed stable from our macroscopic point of view.

Thus, if we look the set of atoms from far enough, the values for certain properties will be somehow averaged. This would be what the Jarzynski equality represents. It gives us the opportunity to see the chair from far away without having to move away.

Furthermore, we can apply the Jensen's inequality on Eq. (**??**) to get

$$\langle W \rangle \geq F_B - F_A, \tag{4.3}$$

which is nothing else but the second law of the thermodynamics. It tells us that for a reversible process, the performed work will equal the change in the free energy. However, for non reversible processes, an extra amount of work is going to be needed, thus increasing the entropy of the system.

Remarkably, the same relation can be proved for the quantum systems, as first demonstrated Tasaki in 2000 [**?**]. We discuss this proof in the next section.

Proof of the quantum Jarzynski equality

Let us assume that our process transitions form state A to state B. The protocol is a little bit different from the classical case and goes like this. Firs we measure the energy of the system in the initial, thermal state. We obtain energy E_n with probability $p_n = e^{-\beta E_n}/Z_A$, coming from Boltzmann factor. The system then undergoes the considered process, that can change the Hamiltonian from the initial one to some final one. The energy of the system is then measured again, resulting in E'_m with conditional probability $p_{m|n} = |\langle \psi'_m | \boldsymbol{U} | \psi_n \rangle|^2$, with $\boldsymbol{U}$ representing the process. Therefore, the joint probability of getting E_n in the first measurement and E'_m in the second one is $p_{m,n} = p_n p_{m|n}$. Let us then compute the average of the exponential of the work, which is defined as $W_{m,n} = E'_m - E'_n$ for each run of the experiment

$$\begin{aligned} \left\langle e^{\beta E_n - \hat{\beta} E'_m} \right\rangle &= \sum_{m,n=1}^{N} p_{m,n} e^{\beta E_n - \hat{\beta} E'_m} = \sum_{m,n=1}^{N} e^{\beta E_n - \hat{\beta} E'_m} \frac{e^{-\beta E_n}}{Z(\beta)} |\langle \psi'_n | U | \psi_m \rangle|^2 \\ &= \sum_{m=1}^{N} e^{-\hat{\beta} E'_m} \frac{1}{Z(\beta)} = \frac{Z'(\hat{\beta})}{Z(\beta)}, \end{aligned} \tag{4.4}$$

which is the mentioned Jarzynski equality (**??**) considering the definition of the free energy in terms of the partition function

A final thing that we would like to mention is that the result shown in Eq. **??** clearly shows the statistical nature of the second law. The second law holds only on average. For a single measurement we can obtain $W_{n,m} < \Delta F$ without violating the second law of thermodynamics. When averaging on a sufficiently high amount of measurements the Jarzynski equality will undoubtedly hold. In the next chapter we will discuss a quantum circuit proposed to simulate Jarzynski equality on real devices.

Chapter 5

Quantum circuit for Jarzynski equality

In this chapter we will discuss a quantum circuit that can be employed in order to study Jarzynski equality in a quantum computer. It is based on the same interferometric technique employed for the simulation of the non-Hermitean Hamiltonians presented in Chapter **??**.

Before starting, let us define the probability distribution associated with the work performed on the system by the process, which is a stochastic variable given its quantum nature. Given its definition in the previous chapter, the rules of statistical physics tell us that the probability distribution is

$$P(W) = \sum_{m,n} p_{m,n} \delta \left(W - (E'_m - E_n) \right). \tag{5.1}$$

The quantum circuit presented in Ref. (**??**) is designed not to measure this probability distribution, but instead its Fourier transform, which is know as the characteristic function

$$\chi(u) = \int P(W) e^{iuW} dW = \sum_{m,n} p_n p_{m|n} e^{iuE'_m} e^{-iuE_n}. \tag{5.2}$$

This is done because it is experimentally difficult to directly measure the work distribution without destroying the initial state when measuring it in the beginning of the process. The idea is to map the information regarding the work distribution into the relative phase of the ancilla system, using the same interferometric technique we discussed before. In the next section we show how this works

The circuit

Let us start by rewriting the characteristic function in a more appropriate way. From Eq. (??) we have

$$\begin{aligned}
\chi(u) &= \sum_{i,j} \frac{e^{-\beta E'_m}}{Z_0} \langle E'_m| \boldsymbol{U} |E_n\rangle \langle E_n| \boldsymbol{U}^\dagger |E'_m\rangle e^{iuE'_m} e^{-iuE_n} \\
&= \sum_{i,j} \frac{e^{-\beta E'_m}}{Z_0} \langle E'_m| \boldsymbol{U} e^{-iu\boldsymbol{H}_i} |E_n\rangle \langle E_n| \boldsymbol{U}^\dagger e^{iu\boldsymbol{H}_f} |E'_m\rangle \\
&= \sum_{i,j} \langle E'_m| \boldsymbol{U} e^{-iu\boldsymbol{H}_i} \boldsymbol{\rho}_0 |E_n\rangle \langle E_n| \boldsymbol{U}^\dagger e^{iu\boldsymbol{H}_f} |E'_m\rangle \\
&= \sum_{j} \langle E'_m| \boldsymbol{U} e^{-iu\boldsymbol{H}_i} \boldsymbol{\rho_0} \boldsymbol{U}^\dagger e^{iu\boldsymbol{H}_f} |E'_m\rangle \\
&= \mathrm{Tr}[\boldsymbol{U} e^{-iu\boldsymbol{H_i}} \boldsymbol{\rho_0} (e^{-iu\boldsymbol{H_f}} \boldsymbol{U})^\dagger]. \qquad (5.3)
\end{aligned}$$

In this equation, $\boldsymbol{H_i}$ and $\boldsymbol{H_f}$ represents the initial (at time 0) and the final (at time τ) Hamiltonians, respectively. Besides, the initial thermal state for the system Qubit is defined as $\boldsymbol{\rho_0} = \frac{e^{-\beta E'_m}}{Z_0}$

Now we will see that there is a quantum circuit that is able to directly measure the characteristic function in the form shown in Eq. (??). The circuit is shown in Fig. ??.

$$\begin{array}{cccccc} |0\rangle_A & \boldsymbol{H} & 1 & \boldsymbol{H} & \langle \boldsymbol{\sigma}_z \rangle, \langle \boldsymbol{\sigma}_y \rangle \\ & & \boldsymbol{\rho_0} & \boldsymbol{G} & \end{array}$$

Figure 5.1: Quantum circuit for measuring the characteristic function associated with the work probability distribution [?].

In the following lines, we will prove that the mentioned circuit effectively fulfills the function of measuring the trace shown in equation (??). As it is claimed in [?], the characteristic function would be measured in the ancillary qubit's final state, which is given by

$$\rho_A = \mathrm{Tr}_S \left[\boldsymbol{H_A G H_A} \left(|0\rangle \langle 0| \otimes \rho_S^0 \right) \boldsymbol{H_A G^\dagger H_A} \right], \qquad (5.4)$$

where the $\boldsymbol{G}$ operator is defined as

$$\boldsymbol{G} = \boldsymbol{O_1} \otimes |0\rangle \langle 0| + \boldsymbol{O_2} \otimes |1\rangle \langle 1|, \qquad (5.5)$$

with

$$\boldsymbol{O_1} = \boldsymbol{U} e^{-i\boldsymbol{H_i} u} \quad \text{and} \quad \boldsymbol{O_2} = e^{-i\boldsymbol{H_f} u} \boldsymbol{U}.$$

So, let us see how the circuit works. If we apply the initial Hadamard gate we get the following state for the ancillary qubit

$$\rho_{AH} = \frac{1}{2} \left(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1| \right).$$

Taking the linearity of the trace into account, we can calculate each of the four terms separately. However, looking at the definition of $\boldsymbol{G}$, it is easy to note that applying it on

the initial state means applying $\boldsymbol{O_1}$ or $\boldsymbol{O_2}$ on the system depending on whether the state of the ancillary qubit is 0 or 1. Of course, if the ancillary qubit state is $|0\rangle\langle 1|$, for example, we will apply $\boldsymbol{O_1}$ from the left and $\boldsymbol{O_2^\dagger}$ from the right. With all this we can compute the result of applying the $\boldsymbol{G}$ operator over the initial state

$$\begin{aligned}\rho_A &= \frac{1}{2}\mathrm{Tr}_S\left[\boldsymbol{H}\,|0\rangle\langle 0|\,\boldsymbol{H}\otimes\left(\boldsymbol{O_1}\rho_S^0\boldsymbol{O_1^\dagger}\right)+\boldsymbol{H}\,|0\rangle\langle 1|\,\boldsymbol{H}\otimes\left(\boldsymbol{O_1}\rho_S^0\boldsymbol{O_2^\dagger}\right)\right]\\ &+ \frac{1}{2}\mathrm{Tr}_S\left[\boldsymbol{H}\,|1\rangle\langle 0|\,\boldsymbol{H}\otimes\left(\boldsymbol{O_2}\rho_S^0\boldsymbol{O_1^\dagger}\right)+\boldsymbol{H}\,|1\rangle\langle 1|\,\boldsymbol{H}\otimes\left(\boldsymbol{O_2}\rho_S^0\boldsymbol{O_2^\dagger}\right)\right]. \qquad (5.6)\end{aligned}$$

In this last equation we also applied the final Hadamard gate to the ancillary qubit. Besides, for those calculations (the ones regarding applying Hadamard gates to the ancillary Qubit), we are going to use the matrix form of the outer products for the sake of compactness.

$$\boldsymbol{H}\,|0\rangle\langle 0|\,\boldsymbol{H}=\frac{1}{2}\begin{pmatrix}1&1\\1&1\end{pmatrix}$$

$$\boldsymbol{H}\,|0\rangle\langle 1|\,\boldsymbol{H}=\frac{1}{2}\begin{pmatrix}1&-1\\1&-1\end{pmatrix}$$

$$\boldsymbol{H}\,|1\rangle\langle 0|\,\boldsymbol{H}=\frac{1}{2}\begin{pmatrix}1&1\\-1&-1\end{pmatrix}$$

$$\boldsymbol{H}\,|1\rangle\langle 1|\,\boldsymbol{H}=\frac{1}{2}\begin{pmatrix}1&-1\\-1&1\end{pmatrix}$$

Furthermore, it is interesting to note that, once applied the partial trace to the terms in (**??**) the first and last system terms would become just one

$$\mathrm{Tr}\left[\boldsymbol{O_1}\rho_S^0\boldsymbol{O_1^\dagger}\right]=1,$$

$$\mathrm{Tr}\left[\boldsymbol{O_2}\rho_S^0\boldsymbol{O_2^\dagger}\right]=1.$$

However, we will still have to deal with the remaining traces. Therefore, for the sake of simplicity we will call $\mathrm{Tr}\left[\boldsymbol{O_1}\rho_S^0\boldsymbol{O_2^\dagger}\right]\to\theta$ and $\mathrm{Tr}\left[\boldsymbol{O_2}\rho_S^0\boldsymbol{O_1^\dagger}\right]\to\theta^*$. As they are both numbers and they are also the complex conjugate of one another. Making all these substitutions the equation (**??**) becomes

$$\rho_A=\frac{1}{4}\left[\begin{pmatrix}1&1\\1&1\end{pmatrix}+\begin{pmatrix}1&-1\\1&-1\end{pmatrix}\theta+\begin{pmatrix}1&1\\-1&-1\end{pmatrix}\theta^*+\begin{pmatrix}1&-1\\-1&1\end{pmatrix}\right], \qquad (5.7)$$

which, by simple algebra, results

$$\rho_A=\left[2\mathbb{1}+\begin{pmatrix}\theta+\theta^*&-\theta+\theta^*\\\theta-\theta^*&-\theta-\theta^*\end{pmatrix}\right]. \qquad (5.8)$$

Here, we can substitute the definitions of the real and imaginary parts of a complex number and separate the matrix into a linear combination of $\boldsymbol{\sigma_z}$ and $\boldsymbol{\sigma_y}$ to obtain

$$\rho_A=\frac{1}{2}\left[\mathbb{1}+\mathrm{Re}(\theta)\boldsymbol{\sigma_z}+\mathrm{Im}(\theta)\boldsymbol{\sigma_y}\right]. \qquad (5.9)$$

Therefore, if we experimentally measure the average expectation value of $\boldsymbol{\sigma_z}$ and $\boldsymbol{\sigma_y}$ we will be measuring the real and imaginary parts of what we called θ. Proving this fact is very simple

$$\langle \boldsymbol{\sigma_z} \rangle = \mathrm{Tr}\left[\boldsymbol{\sigma_z}\rho_A\right] = \frac{1}{2}\mathrm{Tr}\left[\boldsymbol{\sigma_z} + \alpha\boldsymbol{\sigma_z}^2 + \beta\boldsymbol{\sigma_z}\boldsymbol{\sigma_y}\right] = \frac{1}{2}\mathrm{Tr}\left[\alpha\boldsymbol{\sigma_z}^2\right] = \alpha.$$

Here, we have written α to represent the real part of θ and β for the imaginary part. Additionally, the proof for measuring the imaginary part would be analogous to this one.

Notwithstanding we have proven that our circuit measures the real and imaginary parts of some complex number we called θ. The value of θ still has to be checked to see whether it coincides with the trace we are seeking to measure (**??**). By replacing the definitions of $\boldsymbol{O_1}$ and $\boldsymbol{O_2}$ in the definition of θ we obtain

$$\theta = \mathrm{Tr}\left[\boldsymbol{O_1}\rho_S^0\boldsymbol{O_2^\dagger}\right] = \mathrm{Tr}\left[\boldsymbol{U}e^{-i\boldsymbol{H_i}u}\rho_S^0\left(e^{-i\boldsymbol{H_f}u}\boldsymbol{U}\right)^\dagger\right].$$

Which is exactly the trace we wanted. Therefore the circuit does what we expect from it. Nevertheless, the Hamiltonian we are working with will be time dependent. Therefore, the calculation of the evolution operator $\boldsymbol{U}$ is not going to be straightforward. In the next section we will discuss the theoretical aspects of the evolution of time dependent Hamiltonians and how the operator $\boldsymbol{U}$ has to be correctly calculated.

Time dependent Hamiltonians and the Dyson series

In order to simulate the circuit shown in figure (**??**) we need to calculate the form of the time evolution operator for a time dependent Hamiltonian. This is necessary since the thermodynamic process responsible for performing work on the system is usually described by a time-dependent Hamiltonian. To do this, we will begin with the Schrodinger's equation for the evolution operator

$$i\frac{\partial \boldsymbol{U}(t)}{\partial t} = \boldsymbol{H}(t)\boldsymbol{U}(t).$$

By direct integration we obtain

$$\boldsymbol{U}(t) = \mathbb{1} - i\int_0^t \boldsymbol{H}(\xi)\boldsymbol{U}(\xi)d\xi. \tag{5.10}$$

Now we just put this result back into Schrodinger's equation and, by iteration we obtain

$$\boldsymbol{U}(t) = \mathbb{1} - i\int_0^t \boldsymbol{H}(\xi)d\xi + (-i)^2\int_0^t d\xi\int_0^{t'} \boldsymbol{H}(\xi)\boldsymbol{H}(\xi')d\xi' + \ldots, \tag{5.11}$$

which is known as the Dyson equation. We can put this equation into a more elegant way by noting that

- Inside the integrals, the Hamiltonians are not necessarily commuting. Therefore their correct order has to be kept.

- Every subsequent integration limit (t, t', t", ...) has to be lower than the previous one. This means that $t' < t$, $t'' < t'$ and so on.

In order to take care of these observations, we define the time-ordering operator

$$\boldsymbol{T}\left(\boldsymbol{A}(t)\boldsymbol{B}(t')\right) = \begin{cases} \boldsymbol{A}(t)\boldsymbol{B}(t') & \text{if } t' > t \\ \boldsymbol{B}(t')\boldsymbol{A}(t) & \text{if } t > t' \end{cases} \tag{5.12}$$

Next step is to extend all the integration limits to t. However, we will have to take into account how this change in upper limits will affect the integrals, and then compensate these changes in order to not change the final result of the total integral. The easiest case for us to analyse is the third element in the Dyson series where we only have two nested integrals.

$$\int_0^t d\xi \int_0^{t'} \boldsymbol{H}(\xi)\boldsymbol{H}(\xi')d\xi \to \frac{1}{2}\boldsymbol{T}\int_0^t d\xi \int_0^t \boldsymbol{H}(\xi)\boldsymbol{H}(\xi')d\xi = \frac{1}{2}\boldsymbol{T}\left[\int_0^t \boldsymbol{H}(\xi)d\xi\right]^2.$$

First, we note that we had to introduce the time-ordering operator in this equation in order to take care of the fact that the Hamiltonian does not commute with itself in different times. Secondly, the reason why we can extend the integration limits can be understood with the help of Fig. **??**, where the domain of both integrals are displayed. As we can see if we took both integrals from 0 to t instead of enforcing $t' < t$, the result we would get would be the twice since the integration area would be the entire square, while the original one is just the dashed triangle. Therefore, we can compensate the extension in the integration domain by just introducing a factor of 1/2.

The next term in the series has 3 nested integrals, whose integration domain is a tetrahedron. By extending the upper limits of the inner integrals, we are extending the domain of integration from this tetrahedron to a cube, which is 6 times bigger than the original domain. Therefore, we can compensate such change by a factor of $1/6 = 1/(3!)$. Indeed, there is a theorem that proves that the term with n nested integrals will have $n!$ of such simplexes [1]. It follows from this result that we can replace every upper integration limit to t if we multiply the n-th term in the series by the factor $\frac{1}{n!}$ factor. Taking these changes into account, the Dyson series can be written as

$$U(t) = \boldsymbol{T}\left[\sum_{n=0}^{\infty} \frac{(-i)^2}{n!}\left(\int_0^t H(\xi)d\xi\right)^n\right], \tag{5.13}$$

which is nothing but a series expansion for an exponential

$$\boldsymbol{U} = \boldsymbol{T}e^{-i\int_0^t H(\xi)d\xi}. \tag{5.14}$$

Equation **??** is the formal solution of Schrodinger's equation for a time dependent Hamiltonian.

A simple example

In the second section we are going to study the simulations appearing in Ref. [**?**], where the authors implemented in a Nuclear Magnetic Resonance setup the quantum circuit in

[1] Structures like the triangles and the tetrahedron in the case of 2 and 3 integrals, respectively, are called simplexes

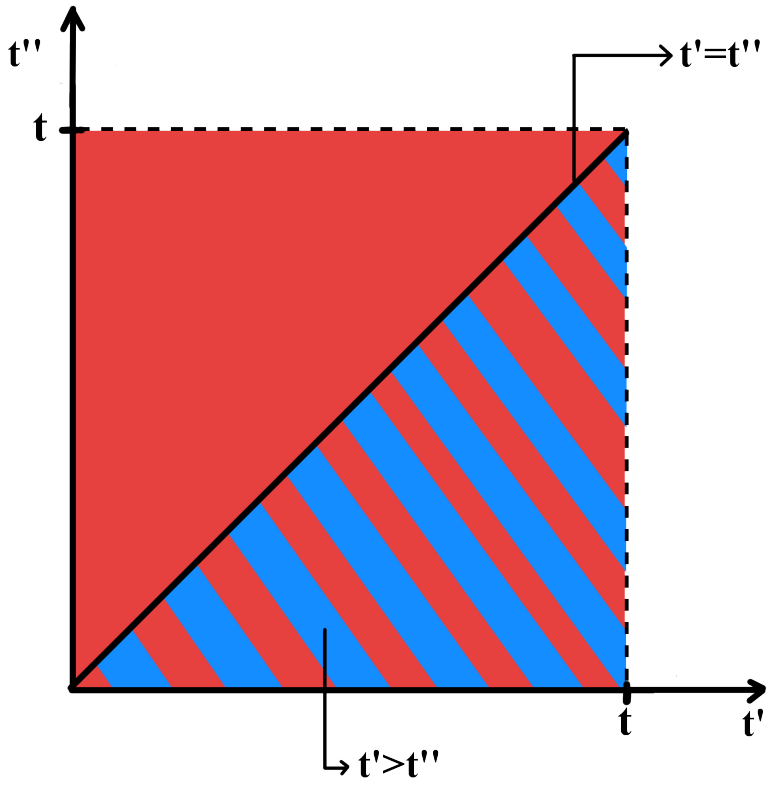

Figure 5.2: Extended domain of integration for the third term in Dyson series.

Fig. ?? to study the work distribution associated with a process governed by a Hamiltonian of in the form

$$\begin{array}{cc} |0\rangle_A & \boldsymbol{L} \quad 1 \quad \boldsymbol{\sigma}_x 1 \ \langle \boldsymbol{\sigma}_x \rangle, \langle \boldsymbol{\sigma}_y \rangle \\ \rho_S & \boldsymbol{R}_0 e^{-iu\boldsymbol{\mathcal{H}}^\alpha(0)} \boldsymbol{U}^\alpha(t) e^{-iu\boldsymbol{\mathcal{H}}^\alpha(\tau)} \boldsymbol{R}_f^\dagger \end{array}$$

Figure 5.3: Quantum circuit responsible for the simulation of the work distribution from [?]. This circuit is a particular case of the more general one shown in Fig.??

$$H(t) = f_x \boldsymbol{\sigma_x} + f_y \boldsymbol{\sigma_y},$$

with

$$f_x = 2\pi\nu(t)\sin(\theta t) \qquad , \qquad f_y = 2\pi\nu(t)\cos(\theta t)$$

and

$$\nu(t) = \nu_1 \left(1 - \frac{t}{\tau}\right) + \nu_2 \frac{t}{\tau}.$$

In these equations, ν_1, θ, and τ are constants.

Since this is a time-dependent Hamiltonian, we need to employ Dyson series (??) in order to build the unitary operation that will be implemented in our simulations. In our simple case in which the system is just a qubit, this can be done analitically.

Let us define the new functions F_x and F_y as the integrals of f_x and f_y, respectively. In terms of these functions, the evolution operator is written as

$$\boldsymbol{U} = \boldsymbol{T} e^{-i(F_x \boldsymbol{\sigma_x} + F_y \boldsymbol{\sigma_y})}. \tag{5.15}$$

Now, by defining the vectors $\boldsymbol{r} = F_x \hat{x} + F_y \hat{y}$ and $\overline{\boldsymbol{\sigma}} = \boldsymbol{\sigma}_x \hat{x} + \boldsymbol{\sigma}_y \hat{y}$, we can write

$$\boldsymbol{r} \cdot \overline{\boldsymbol{\sigma}} = F_x \boldsymbol{\sigma_x} + F_y \boldsymbol{\sigma_y}. \tag{5.16}$$

Additionally, we can always rewrite $\boldsymbol{r}$ as $r\hat{r}$, with r being the norm of the vector $\boldsymbol{r}$, while $\hat{r}$ is a unit vector parallel to $\boldsymbol{r}$. Finally, we can re-express the whole exponential as

$$\hat{U} = \boldsymbol{T} e^{-ir(\hat{r} \cdot \boldsymbol{\sigma})} = \boldsymbol{T} \left(\cos(r) \mathbb{1} - i \left(\hat{r} \cdot \boldsymbol{\sigma} \right) \sin(r) \right). \tag{5.17}$$

However, there is nothing in the right had side of this equation that needs to be time-ordered, since the time dependence lies only inside real-valued functions, which commutes at different times. Therefore, the time-ordering operator is not necessary.

Once we computed the operator for the time evolution with our Hamiltonian, there is still one task left, beyond putting all the gates together. We have to prepare the initial state of the system in a thermal distribution

$$\rho_S = \frac{e^{-\beta H(0)}}{Z_0} \quad \text{with} \quad Z_0 = Tr[e^{-\beta H(0)}]. \tag{5.18}$$

The initial state of the system of interest plus the ancillary one is then given by

$$|i\rangle = |0\rangle_A \langle 0|_A \otimes \rho_S. \tag{5.19}$$

Remember that a few lines back we proved that we had to measure the expectation values of $\langle \boldsymbol{\sigma}_z \rangle$ and $\langle \boldsymbol{\sigma}_y \rangle$ of the ancillary Qubit in order to get the real and imaginary parts of the characteristic function associated with the work probability distribution (equation **??**). Nevertheless, as we are taking Ref. [**?**] as the reference for the simulation, we simulate the circuit from Fig. **??**. Therefore, in this case we will have to measure the values of $\langle \boldsymbol{\sigma}_x \rangle$ and $\langle \boldsymbol{\sigma}_y \rangle$. The reason for this is the slight difference between circuits **??** and **??**. Considering the entire circuit, we need to measure the operators

$$\langle \boldsymbol{\sigma}_x \rangle = \mathrm{Tr}\left((\boldsymbol{\sigma}_x \otimes \mathbb{1}) \rho \right) \quad \text{and} \quad \langle \boldsymbol{\sigma}_y \rangle = \mathrm{Tr}\left((\boldsymbol{\sigma}_y \otimes \mathbb{1}) \rho \right). \tag{5.20}$$

The results of our simulation is plotted against u (the conjugate variable to work) in Fig. **??** and Fig.**??**, while its Fourier transform, the reconstructed work probability distribution, is shown in Fig. **??**. As we can see, $\boldsymbol{\sigma}_y$ varies more quickly with the temperature than $\boldsymbol{\sigma}_x$ does.

Jarzynski equality from the characteristic function

Up to now, we have revisited the Jarzynki equality and then measured the characteristic function of work performed on some system. Besides, it has been stated that the point of measuring such characteristic function was to avoid destroying the state of the

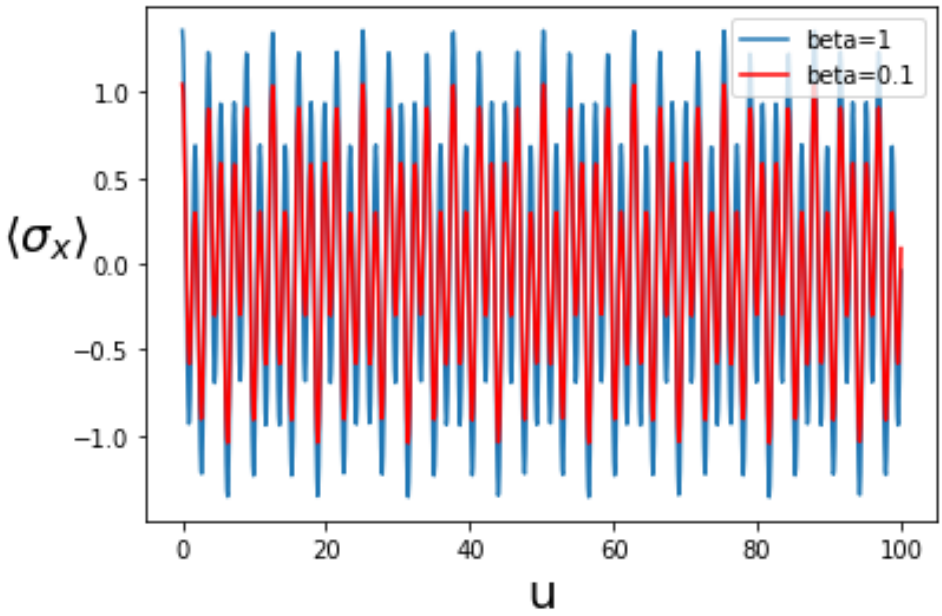

Figure 5.4: In this figure we can see the average value of $\boldsymbol{\sigma_x}$ against u, which is the conjugate variable of work. The average values has been plotted for two values of the temperature β

system when measuring energy. However, there is an extra reason, we can provide an experimental[2] benchmark to test whether Jarzynski equation holds.

As a matter of fact, we have proven the following Jarzynski equality in equation (**??**)

$$\left\langle e^{-\beta W} \right\rangle = \frac{Z_\tau}{Z_0}. \tag{5.21}$$

Furthermore, because of the definition of the characteristic function as the Fourier transform of the work probability distribution

$$\chi(u) = \int P(W) e^{iuW} dW = \left\langle e^{-iuW} \right\rangle,$$

we note that it is also the definition of the average value of e^{iuW}. Therefore, setting $u = i\beta$ we can get exactly the RHS from Jarzynski equality given in Eq. (**??**)

$$\chi(u = i\beta) = \left\langle e^{-\beta W} \right\rangle = \frac{Z_\tau}{Z_0}.$$

Consequently, as long as we are able to calculate the partition functions for the system at different times, we will also be able to check Jarzynski equality.

This very same verification was carried out in Ref. [**?**], where its authors tested Jarzynski equality using the circuit shown in Fig. **??**, obtaining positive results. Thus, experimentally demonstrating how the Jarzynski fluctuation theorem holds under the circumstances we stated before in this thesis.

[2]Even though in this case it would be a simulation.

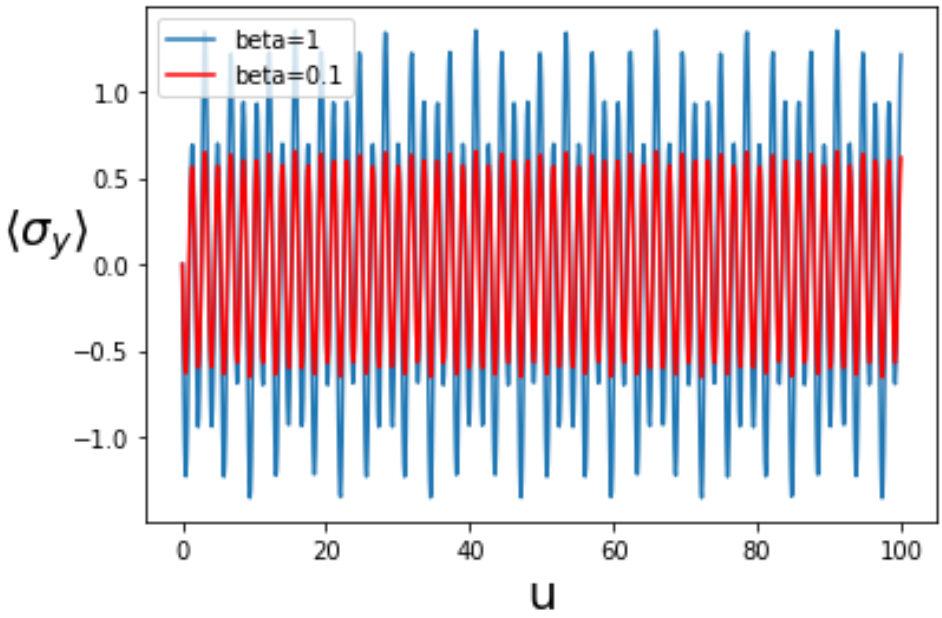

Figure 5.5: In this figure we can se the average value of $\boldsymbol{\sigma_y}$ agains u, which is the conjugate variable of work. The average values has been ploted for two values of the temperature β

Chapter 6

Conclusions

In this thesis we considered two main areas. First we explored additional possibilities above and beyond Hermitian Hamiltonians within the so called $\mathcal{PT}$ symmetric formulation of quantum mechanics, which allows the Hamiltonians to be non-Hermitian while keeping the reality of the energy spectrum and the unitarity of time evolution.

Section **??** makes clear that it is not possible to directly implement non Hermitian Hamiltonians in quantum computers. This is the reason why we have to use extra ancillary systems (Qubit) in order to build a quantum circuit that is able to simulate the behavior of a $\mathcal{PT}$ symmetric Hamiltonian in usual quantum computers. This quantum circuit was originally described in Ref. [**?**].

Beyond the systems with a $\mathcal{PT}$ symmetric Hamiltonian, there was another matter of interest for us in this thesis; it was quantum thermodynamics. We analysed how a quantum circuit can be used to study the characteristic function associated with the probability distribution of the work performed on a quantum system. In Sec. **??** we showed how such circuit can be used in the context of the Jarzynski equality, which is one of the most important fluctuation theorems to date.

It is interesting to observe that both circuits just mentioned are based on the same interferometric technique. The first one, used in the case of non-Hermitian Hamiltonians, uses interferometry to map the $\mathcal{PT}$ evolution into the phase of the auxiliary system, while the second one employs the interferometry in order to map the information about the work probability distribution into the phase of the ancillary system. Therefore, both parts of the thesis are deeply linked.

This fact lead us to think about the possibility of merging the two fields discussed above. By merging both quantum circuits discussed in this thesis, it should be possible to study, in a quantum computer, thermodynamic processes, and the associated fluctuation relations, driven by non-Hermitian Hamiltonians. It should be possible, among other things, to observe a breakdown of the fluctuation relations when the $\mathcal{PT}$ symmetry is broken. Also, due to the deep link between Jarzynski equality and the second law of thermodynamics, this could provide some new insights into the quantum extension of the laws of thermodynamics. This line of investigation is certainly very interesting.