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**Thermodynamic Uncertainty
Relation: A Phase Space Perspective**

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LETÍCIA LIRA TACCA

**Thermodynamic Uncertainty
Relation: A Phase Space Perspective**

Dissertação apresentada ao Programa de Pós-Graduação em Física, do Instituto de Física, da Universidade Federal de Goiás (UFG), como requisito para obtenção do título de Mestre em Física.

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Aos 14 dias do mês de fevereiro de 2022, a partir das 09h00min, por meio de videoconferência, realizou-se a sessão pública de Defesa de Dissertação intitulada “Thermodynamic uncertainty relation: a phase space perspective”. Os trabalhos foram instalados pelo Orientador, Professor Doutor Lucas Chibebe Céleri (IF/UFG), com a participação dos demais membros da Banca Examinadora: Professor Doutor Miled Hassan Youssef Moussa (IFSC/USP), membro titular externo; e Professor Doutor Celso Jorge Villas-Bôas (DF/UFSCAR), membro titular externo. Durante a arguição, os membros da banca não fizeram sugestão de alteração do título do trabalho. A Banca Examinadora reuniu-se em sessão secreta a fim de concluir o julgamento da Dissertação, tendo sido a candidata aprovada pelos seus membros. Proclamados os resultados pelo Professor Doutor Lucas Chibebe Céleri, Presidente da Banca Examinadora, foram encerrados os trabalhos e, para constar, lavrou-se a presente ata que é assinada pelos membros da Banca Examinadora, aos 14 dias do mês de fevereiro de 2022.

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“Somewhere, something incredible is waiting to be known.”

Carl Sagan

Abstract

Thermodynamic uncertainty relations describe a trade-off between energy and precision. By energy here, we understand dissipated energy in the thermodynamic context, in terms of entropy production. By precision, we mean a measure of the relative uncertainty associated with an observable of interest. It is a fundamental lower bound that connects thermodynamics and information theory and can be extended to the quantum mechanical approach. In this dissertation, we build a thermodynamic uncertainty relation in the quantum mechanical phase space, by using the coherent state representation and the Husimi Q-function, which allows us to analyze an interface between classical and quantum physics. The observable considered was the Husimi current that characterizes the phase space flow. First, we define the Fisher information in the phase space and, from this, we derive the Cramér-Rao bound (CRB), which is an inverse relation between the variance of the estimator of some variable and the Fisher information. After this, by means of the connection between Fisher information and relative entropy and, between relative entropy and the thermodynamic entropy production we derive the thermodynamic uncertainty relation in the phase space.

Keywords: Quantum physics, Information theory, Thermodynamics, Uncertainty relations, Phase space.

Resumo

Relações de incerteza termodinâmicas descrevem uma troca entre energia e precisão. Por energia, entendemos energia dissipada no contexto termodinâmico, em termos de produção de entropia. Por precisão, queremos dizer uma medida da incerteza relativa associada a um observável de interesse. É um limite inferior fundamental que conecta a termodinâmica e a teoria da informação e pode ser estendido à abordagem da mecânica quântica. Nesta dissertação, construímos uma relação de incerteza termodinâmica no espaço de fases da mecânica quântica, usando a representação de estados coerentes e a função Q de Husimi, que nos permite analisar uma interface entre a física clássica e a quântica. O observável considerado foi a corrente de Husimi que caracteriza o fluxo no espaço de fase. Primeiramente, definimos a informação de Fisher no espaço de fase e, a partir disso, derivamos o limite de Cramér-Rao (CRB), que é uma relação inversa entre a variância do estimador de alguma variável e a informação de Fisher. Em seguida, por meio da conexão entre a informação de Fisher e a entropia relativa e, entre a entropia relativa e a produção de entropia termodinâmica, derivamos a relação de incerteza termodinâmica no espaço de fase.

Palavras-chave: Física quântica, Teoria da informação, Termodinâmica, Relações de incerteza, Espaço de fase.

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List of Abbreviations

TUR	Thermonynamic Uncertainty Relation
FT	Fluctuation Theorem
NESS	Non-equilibrium Steady State
LES	Local Equilibrium State
SSM	Steady States Manifold
Finf	Fisher information
CRB	Cramer-Rao Bound
BCH	Baker-Campbell-Hausdorff formula

Dedicado a minha Vó Norberta.

Chapter 1

Introduction

THE relation between energy cost and precision is intrinsic to measurement processes. By energy here, it is understood the thermodynamic cost associated with some physical process [1, 2, 3], and precision has a purely statistical meaning: it is a measure of relative uncertainty of some specific parameter associated with this process and/or system, i.e., a measure of statistical variability [4]. Naturally, there are physical limits to measuring physical variables, in the sense that there is no way to measure a certain parameter with maximum precision without having an energy cost related to it. That is, there is an uncertainty relation between the energy consumption of a given process and its measurement precision, and this is a thermodynamic relation that can be fully characterized with well-established theoretical tools [5], and that has direct application in quantum metrology [6], where increasing the precision of a measurement means, as a consequence, decreasing the energy efficiency of technological devices of wide application [7, 8], thus increasing the dissipated energy.

At the core of this relation is the concept of *entropy* and the second law of Thermodynamics [9]. According to this fundamental law, entropy, which here is understood to be the thermodynamic cost itself (in terms of dissipated energy) [10], always increases in a physical process. Here, since we will be dealing with quantum systems, we are considering the average over an ensemble of realizations of the process when making such statement. This is due to the fact that, when we take the second law into quantum contexts, there may be microscopic fluctuations in which this law can be violated [11, 12], as we will see in more detail in the next chapter. By fluctuations here, in a general context, we mean significant deviations from an average value of an arbitrary variable being measured. It can occur for both classical and quantum systems, however, in macroscopic systems, such fluctuations are so small that they can be ignored. In the quantum context, fluctuations can refer to random changes in the amount of energy of a given state [13], for instance. From the thermodynamic point of view, when the fluctuations are large enough to be considered, there is a probability that the entropy production decreases, and this

is what is called a "violation" of the second law. However, on average, the second law is expected to hold, telling us that entropy changes are always non-negative.

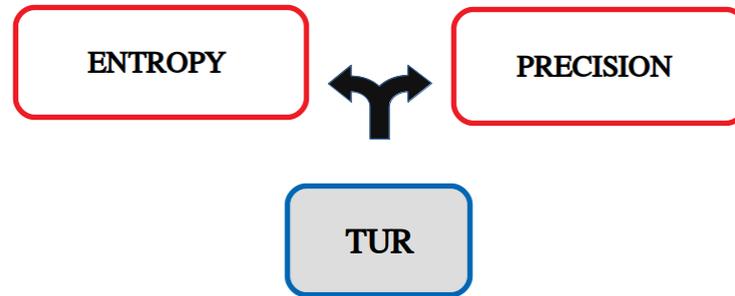


FIGURE 1.1: TUR is a trade-off relation between energy cost and precision.

To this trade-off relation between entropy production and measurement precision is given the name of thermodynamic uncertainty relation (TUR). The first TUR derivation date back to recent years and was carried out in the context of quantum metrology [1]. Latter on, further developments were observed, in the context of stochastic processes applied to biological systems [14] as well as other types of systems [15]. It was noted that TUR also applied to different contexts, both classical and quantum [1, 16], albeit with minor modifications. This can be considered an emerging theory in quantum thermodynamics, and with direct implications for the development of more efficient measuring techniques. What we intend to do in this work is to explore the possibility of developing a TUR by considering the phase space description in the quantum context [17], and connecting it to information theory and quantum optics. The reason behind this connection will become clear soon.

As well as the famous Heisenberg uncertainty relation [18], which describes indeterminacy in quantum mechanics, and establishes a minimum value for the product of the variances of the parameters P (momentum) and Q (position) that draw the phase space, the thermodynamic uncertainty relations provide us with a threshold for the average entropy production due to the variance of some observable, which can be, for example, an average fluctuation of some current. Such a current can be of particles, electrical charges, heat, or even of an arbitrary probability current [19, 20]. The physical meaning of the current will depend on the system at hand and the process related to it. However, whichever the case, the current can be determined in terms of its fluctuations, and with the description of the flow of this current, a perspective of the evolution of the system and the associated energy dissipation can be obtained. Our goal is to understand if it is possible to use the quantum mechanical phase space perspective to build a TUR that bounds probability current variances,

and how this is related with the entropy production and the thermodynamics of a quantum system.

With that in mind, we must fully understand the context in which we will develop our TUR. When we say terms like “flow”, “current”, and “phase space”, it is natural that we first think in classical terms, as these are derived concepts and used widely in classical physics [21]. In fact, one of the firsts derivations of TURs were in classical systems, which although they were stochastic (randomly determined) were also macroscopic and with their thermodynamics well determined. However, trying to describe physical concepts in the quantum perspective is a natural way of going deeper into basic theory. Seeking to understand the TURs from a quantum point of view and comparing them to the classical case, becomes an essential and complementary activity for a more complete foundation of the theory. There is already extensive literature on the subject, including derivations of quantum TURs for several systems, as we will see in detail in Chapter 2. For our case, however, we will describe a *quasiprobability* flow for the phase space [22], and from the latter obtain a TUR that describes the thermodynamic cost of the current associated with the Husimi’s function [23] in this space. Why we use quasiprobability functions in this approach and what this means will become clear in Chapter 3, however, it is the price we pay for describing quantum mechanics in phase space.

Moreover, there are some very important details to be taken into account: how to describe the phase space and its fluxes in quantum terms, and why to use phase space? Which quantum concepts should be defined and which mathematical formalism should be used? What about the systems that should be considered? How to interpret all of this physically? Why is it interesting to elaborate a TUR for this flow? What are the future applications and areas of interest?

All these questions and many others arose naturally during the development of this work and served as a guide for the structure of the theory to be presented. Therefore, this dissertation is organized to follow the path developed throughout the research period. In Chapter 2, a general approach is made about the TURs, from their connection with fluctuation and dissipation theorems to the initial description in classical contexts and the subsequent quantum development, in the context of out-of-equilibrium steady states. In Chapter 3, the theoretical foundation of the phase space description of both classical and quantum mechanics is presented, with special focus on the description of current flow in terms of the Husimi representation, which is one of the possible descriptions of the phase space in quantum mechanics. The choice for the phase space representation and the Husimi’s function in this work was due to its unique characteristics that allow us to visualize the theory

under a brand new perspective, and it has the potential of finding new concepts directly linked with other areas of physics, such as chaotic systems, for instance. With the theoretical tools developed in the two previous chapters, in Chapter 4 the thermodynamic uncertainty relation for the Husimi flow is developed, and we discuss its implications. In Chapter 5, we take an overview of all the work and discuss the project's prospects. In the Appendix, we show details of the calculation of specific topics in the main text.

Chapter 2

Thermodynamic Uncertainty Relations

THERMODYNAMIC uncertainty relation (TUR) refers to an intrinsic feature of the process of measuring a physical quantity, which is the fact that there is a dispersion of computed values for a given variable, or an "uncertainty", which is directly linked to an energy cost due to the measurement process [24]. It is a trade-off relation between entropy and precision, and it is essential for understanding not only the physics of the problem at hand, but mainly for understanding the mechanisms used in experimental techniques. This relation was considered in many situations. Barato and Seifert, considering the case of biomolecular processes [14], proposed a non-equilibrium principle, a TUR that describes a fundamental bound in the dissipation that regulates fluctuations. After that, several other works were carried out attesting to the validity of the TUR [25], including analytical and numerical calculations [26, 27]. Generalizations of the TUR were also obtained in other systems and contexts [1, 28, 29], and the applications already include insights into a large variety of scenarios, for instance, in quantum devices [30], molecular motors [31], and biochemical sensing [32]. To better understanding the main concepts used to derived the TUR, one needs to make a brief contextualization of the systems and processes involved in it.

2.1 Non-equilibrium thermodynamics

Fundamentally, thermodynamics is the area of physics responsible for describing and analyzing processes and systems that involve energy exchange in the form of heat and work [10]. More than that, in addition to being concerned with temperature measurements and energy efficiency for applications in thermal machines, it is an essential tool in the study of the behavior of matter and its transformations. The fundamental laws of thermodynamics explain the exchange of heat between bodies and systems with the environment and how we can control this in order to get

useful work [33]. The application of the thermodynamic theory in different areas of interest provides a better understanding of physical concepts such as *equilibrium* and *efficiency*, and in the context of the information theory, we can also define the entropy associated with acquiring information [34].

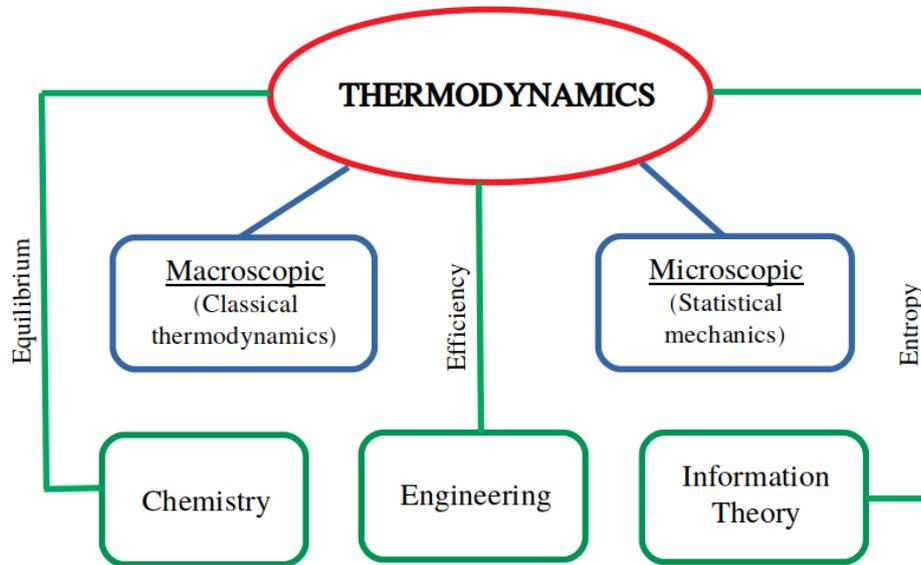


FIGURE 2.1: Scheme for the different approaches in thermodynamics and some applications.

At the macroscopic level, we cannot observe violations of the fundamental laws of thermodynamics due to the statistical nature of thermodynamic systems. As the number of molecules increases, the order of magnitude of the degrees of freedom involved will be so large that, statistically speaking, the chances of violating the second law are almost non-existent. However, at the microscopic level, where systems are small enough for fluctuations to matter, there is a chance of observing such violations [11, 35]. It is important to note here that this is not a violation of the fundamental laws of physics, but only a statement of the statistical nature of the second law of thermodynamics.

When such fluctuations become important, we say that we have a *stochastic process*, that is, a random process. This process is characterized by random variables that can assume numerical values of a specific system that changes over time. For instance, the movement of a gas molecule, or an electrical current fluctuation is some of the stochastic processes often studied in Physics and Chemistry [36]. Also, this mathematical concept has applications in many different areas, such as Ecology and the study of populations dynamics [37], cell biology [38], neuroscience and the study of neuronal models [39], computer science [40], and information theory [41], among others. In thermodynamics, stochastic processes play a central

role in describing small systems, in particular when they are away from thermal equilibrium [42, 43].

2.1.1 Irreversibility and the second law

A fundamental characteristic of non-equilibrium thermodynamics is the *irreversibility* of its processes [44]. Irreversibility refers to the property of a system to change from a certain initial state to another state, but without being able to return to its initial state. In the case of systems where the equations of motion or trajectories are known, their anti-trajectories are also known, that is, their reverse trajectories in time, which are also solutions to the equations. When the probabilities of observing the trajectories are equal to the probabilities of their respective anti-trajectories, we say that the system is reversible. Otherwise, if these probabilities are different, the system is said to be irreversible.

The second law of thermodynamics states that in a system in thermal equilibrium, entropy (which is an extensive property defined in terms of the change in the amount of heat by the absolute temperature) always increases, and is only constant if all processes are reversible [10, 33]. Then, for a system that evolves irreversibly, the entropy production is non-negative.

Away from equilibrium, heat losses occur between the system and the environment, also called a *thermal bath*. In a thermal equilibrium situation, this does not happen, as the probability of absorbing or losing heat is identical. In fact, this is how statistics defines the concept of thermal equilibrium, that is, if we calculate the ratio between the probabilities of energy exchanges, we have that $P(Q)/P(-Q) = 1$, where $P(Q)$ denotes a probability that the system exchanges an amount of Q of heat. Under non-equilibrium conditions, this ratio tends to be quite different, as we will see soon.

2.1.2 Fluctuation Theorems

For small systems, where fluctuations matter, the second law has limitations and we need other ways to better describe the reversibility of these systems. The fluctuation theorems (FT) developed in recent decades [45] are fundamental tools in the analytical description of non-equilibrium states and show how the irreversible dynamics of microscopic systems arise from reversible processes, which for a long time has been known as Loschmidt's paradox [46]. Although several fluctuation theorems have been proposed over the last few years, in this dissertation we will turn our attention to two of them, which are directly applicable to the development of our work: the Evans-Searles FT [47, 48], which seeks to generalize the second

law to small systems that can evolve in a far from equilibrium processes; and the Crooks FT [49, 50], which describes fluctuations from a free energy exchange perspective. Both are theorems that quantify the irreversibility that emerges from the reversible equations of motion of a system and are essential in the applicability of thermodynamic concepts in a range of nanotechnologies of interest [51].

The Evans-Searles FT

In 1993, Evans *et al.* [11] developed a fluctuation theorem that quantitatively described violations of the second law of thermodynamics, obtaining the probability that there would be a dissipative flow in the opposite direction to that predicted. In other words, the theorem predicted observations of the violation of the second law violation for small systems over a short time scale. According to this FT, when calculating the ratio between the probabilities of observing trajectories in phase space¹, of a certain duration t , in both temporal directions, with an entropy production Σ_t , we have that

$$\frac{P(\Sigma_t = A)}{P(\Sigma_t = -A)} = \exp(A), \quad (2.1)$$

where A is an arbitrary number, and the entropy production scales with system size and time t . Thus, one can show that as trajectory duration becomes longer or system size gets larger, the chance of observing anti-trajectories is exponentially smaller, and it becomes likely that the system appears time irreversible, as the second law states.

The Crooks FT and Jarzynski's Equality

Crooks [49, 50] obtained a fluctuation theorem that describes processes that start in a certain equilibrium state A , and after being removed from this state by the action of an external agent, it ends in a non-equilibrium state B . This is known as the *forward* process. The *reverse* process happens when the system starts in a equilibrium state B and ends in a non-equilibrium state A , following the reverse protocol. Both processes last for a time t . In such conditions, the Crooks FT states that

$$\frac{P_f(W)}{P_r(-W)} = \exp\left(\frac{W - \Delta F}{k_B T}\right). \quad (2.2)$$

Here, k_B is Boltzmann's constant, T is the initial temperature of the system, $P_f(W)$ and $P_r(-W)$ are the probabilities of observing the forward and reverse processes, respectively. The free-energy change between equilibrium states A and B is $\Delta F = F_B - F_A$. For reversible paths, the ratio in (2.2) is equal to 1, and $W = \Delta F$, as

¹See Chapter 3 for phase space definitions.

expected in classical thermodynamics. Also, if we compute the average over the ensemble of realizations, one can show that

$$\langle e^{-W/k_B T} \rangle = e^{-\Delta F/k_B T}, \quad (2.3)$$

which is known as Jarzynski's equality and was first proved by Jarzynski in 1997 [52], before the derivation of the Crooks FT. Other FTs have been reported since then, and they differ from each other according to their initial conditions and details in the system's dynamics [47, 53, 54, 55, 56].

From the equality in (2.3) and using the Jensen's inequality [57, 58], $\langle e^x \rangle \geq e^{\langle x \rangle}$, we get the inequality related to the second law of thermodynamics in terms of free energy and work

$$\langle W \rangle \geq \Delta F, \quad (2.4)$$

where the difference $\langle W \rangle - \Delta F$ is the *dissipated work*, W_{diss} , responsible for increasing the entropy during an irreversible process.

2.2 Information theory and thermodynamics

As mentioned earlier, the concept of entropy in thermodynamics can be defined as the rate of heat and temperature, also called an increase in the disorder of a system. However, entropy can be defined in different contexts in conceptually different ways. In information theory, entropy is the measure of how much we don't know about a certain random variable, that is, the uncertainty we have about it. At first glance, this concept seems a bit strange, as what does it mean to "measure how much you don't know"? However, the very definition of "information" is connected to this. Acquiring information can have different meanings, depending on the situation, but generally, information is something new that brings us knowledge about a certain subject. Furthermore, if we discuss in physical terms, this process requires a thermodynamic cost [1]. Mathematically, information can be described in terms of probability distributions, and these also define the information entropy [41].

Definition 1. Let p be a probability distribution linked to a continuous random variable. The information entropy associate with p is defined as [59]

$$I[p] \equiv - \int p \ln p \, dx, \quad (2.5)$$

where x is some relevant integration variable (or set of variable).

This definition is also known as *Shannon's entropy* in honor to Claude Shannon [60], and it essentially measures the amount of information related to some random variable, or its *uncertainty*. The relation between I and thermodynamics is given by

$$I[p^{eq}] = \frac{S}{k_B}, \quad (2.6)$$

where S is the thermodynamic entropy, and p^{eq} describes the thermodynamic equilibrium distribution.

2.2.1 Relative Entropy and Dissipation

In case we have two probability distributions, the measure of information we want to obtain, in the context of thermodynamics, will be the *relative entropy* between them, which is defined as how distant one function is from the other [41, 61]. Also, this information-theoretic measure relates directly to dissipated work, $W_{diss} = W - \Delta F$.

Definition 2. Consider two normalized probability distributions, $p(x)$ and $q(x)$, in the same space of variables. The measure that quantifies how much one distribution differs from the other is defined by [62]

$$D[p|q] = \int p \ln \left(\frac{p}{q} \right) dx \geq 0, \quad (2.7)$$

and it is called *relative entropy* (or *Kullback-Leibler divergence*).

In the case of distributions of trajectories, if P_F and P_R represent the forward and reverse processes, respectively, we can apply the Crooks' fluctuation theorem in (2.2) to obtain the relative entropy $D[P_F|P_R]$ that quantifies how the system's evolution during one process differs from that during the other. Therefore, it follows that

$$D[P_F|P_R] = \frac{W_F^{diss}}{k_B T}, \quad (2.8)$$

where $W_F^{diss} = \langle W \rangle_F - \Delta F$ is the mean value of dissipated work during the forward process.

Relative entropy is asymmetric, i.e., $D[p|q] \neq D[q|p]$. However, it is possible to quantify thermodynamic irreversibility through other symmetric measures that relate to different relative entropies. For instance, in Ref. [63], the authors discuss the use of two symmetric measures and work fluctuation relations to determine the time asymmetry of single-molecule RNA, and then understanding how the thermodynamic arrow of time arises from an underlying time-reversible dynamics.

By analogy with the trajectories in phase space, we can also draw the forward and reverse processes as shown in Fig. 2.2, where there is a deterministic dynamics with phase space point (q, p) at time t . The initial and final phase space points are (q_0, p_0) and (q_1, p_1) , respectively. The time-reversed protocol starts from $(q_1, -p_1)$, goes through $(q, -p)$, and gets into $(q_0, -p_0)$. The notation for the time t is set to be the forward time in both scenarios.

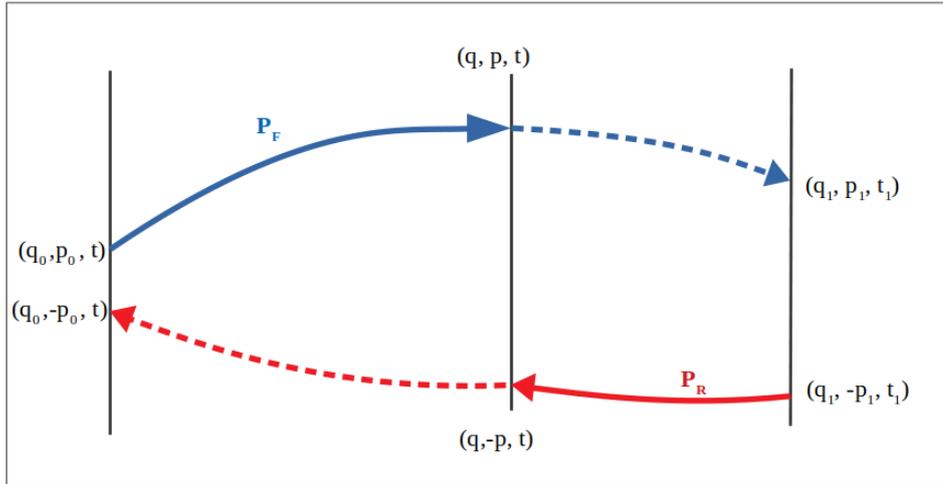


FIGURE 2.2: Forward (blue) and reverse (red) trajectories from the phase space perspective, with space-time coordinates.

2.2.2 Entropy production

Now let us define the *entropy production* and how it is related to the second law. From the first law of thermodynamics [10], we have that

$$\Delta U = W + Q, \quad (2.9)$$

where U is the internal energy of the system. This relation can also be written in terms of the Helmholtz free energy, $F = U - TS$. Thus,

$$\frac{W - \Delta F}{T} = \Delta S - \frac{Q}{T} = \Delta S_{tot}, \quad (2.10)$$

where ΔS_{tot} is the total entropy change of the system and environment. For microscopic systems, we will assume that for a thermodynamic process, Eq. (2.10) holds. In order to obtain the fluctuations of entropy production, we apply the Evans-Searles' FT in Eq. (2.1) to a system that evolves from an initial equilibrium state to a non-equilibrium state during a time $t > 0$. If $P(\Delta s)$ is the probability distribution

of the entropy produced, we have that

$$\frac{P(+\Delta s)}{P(-\Delta s)} = e^{\Delta s}. \quad (2.11)$$

We can further integrate this last expression in order to obtain a fluctuation theorem in the form

$$\langle e^{-\Delta s} \rangle = 1, \quad (2.12)$$

and from the exponential function properties, we get the second law

$$\langle \Delta s \rangle \geq 0. \quad (2.13)$$

If we consider a system that evolves into a non-equilibrium state in the long time limit, one can denote $\sigma = \Delta s/t$ as the *entropy production rate*, and then the steady-state fluctuation theorem of Gallavotti & Cohen [64, 64] states that

$$\lim_{t \rightarrow \infty} \frac{1}{t} \ln \frac{P_t(+\sigma)}{P_t(-\sigma)} = \sigma, \quad (2.14)$$

where we set $k_B = 1$. Integrating this last expression, we obtain

$$\lim_{t \rightarrow \infty} \frac{1}{t} \ln \langle e^{-\sigma t} \rangle_t = 0, \quad (2.15)$$

and, therefore

$$\langle \sigma \rangle_t \geq 0, \quad (2.16)$$

which is the statement that entropy production rate must be positive.

2.3 Quantum mechanics perspective

So far we have seen the application of fluctuation theorems to small classical systems, which have direct experimental applications in studies of biomolecules and related subjects. However, to better understand microscopic phenomena, we must analyze fluctuations from a quantum point of view, as this is relevant in various applications of quantum computing devices, such as NMR² experiments [65], superconducting qubits [66], trapped ions [67], among others. Quantum fluctuation theorems have been largely studied over the past few years, and there is extensive literature ranging from isolated quantum systems described by unitary dynamics [68] to open quantum systems [69], and even quantum field theory [70]. In this

²NMR - Nuclear Magnetic Resonance.

section, we will focus our attention on the quantum formulation of the fluctuation theorems applicable to isolated systems [71].

2.3.1 Background on Quantum Mechanics

Let us begin with a brief review on basic concepts of quantum mechanics. The quantum systems we are dealing with are described by a Hilbert space \mathcal{H} . Here, we are going to consider just finite-dimensional systems.

Quantum States and Observables

We can define a quantum state that can be characterized by the density operator $\rho \in \mathcal{B}(\mathcal{H})$, where $\mathcal{B}(\mathcal{H})$ represents the bounded operators acting on Hilbert space \mathcal{H} , satisfying $\rho \geq 0$ and $\text{Tr}(\rho) = 1$. When the density operator is pure, we have [72]

$$\rho = |\psi\rangle\langle\psi|, \quad |\psi\rangle \in \mathcal{H}, \quad (2.17)$$

and $|\psi\rangle$ is called a state vector fulfilling the condition $\langle\psi|\psi\rangle = 1$. The positivity property of ρ means that $\langle\psi|\rho|\psi\rangle \geq 0$ for any $|\psi\rangle \in \mathcal{H}$.

Physical quantities (observables) are described by Hermitian operators $A \in \mathcal{L}(\mathcal{H})$, with $\mathcal{L}(\mathcal{H})$ representing the space of linear operators acting on \mathcal{H} . The spectrum decomposition theorem states that

$$A := \sum_k a_k |\varphi_k\rangle\langle\varphi_k|, \quad (2.18)$$

where $\{|\varphi_k\rangle\}$ is an orthonormal basis of \mathcal{H} . The measurement of the observable A results in the outcome a_k . Using the Born rule [73], we have that the probability of obtaining a_k is given by

$$p(k) := \langle\varphi_k|\rho|\varphi_k\rangle, \quad (2.19)$$

where ρ refers to the quantum state. This last relation also satisfies

$$\sum_k p(k) = \text{Tr}(\rho) = 1. \quad (2.20)$$

The average over all the outcomes is then given by

$$\langle A \rangle := \sum_k p(k) a_k = \text{Tr}(A\rho). \quad (2.21)$$

If we have a pure state as the expression in (2.17), we get

$$p(k) = |\langle \psi | \varphi_k | \psi \rangle|^2, \quad (2.22)$$

$$\langle A \rangle = \langle \psi | A | \psi \rangle. \quad (2.23)$$

Furthermore, if there is an interaction of two systems, R and S , their composite system is described by the tensor product space $\mathcal{H}_{RS} = \mathcal{H}_R \otimes \mathcal{H}_S$. Thus, $\rho^{RS} \in \mathcal{B}(\mathcal{H}_{RS})$ will be the density operator of the composite system.

Quantum dynamics

The time evolution of the density operator differs depending on which system we are concerned. For instance, for an isolated quantum system, the evolution is said to be an unitary evolution, because the evolution operator U acting on the initial state is unitary, i.e., $U^\dagger U = U U^\dagger = I$, where $U \in \mathcal{U}(n)$, the space of unitary matrices of dimension n . In this case, a density operator evolves as

$$\rho \rightarrow U \rho U^\dagger \quad (2.24)$$

This automatically preserves positivity and the trace of ρ . If a closed system evolves during a certain time t , the unitary operator is given by

$$U \rightarrow U(t) = e^{-iHt/\hbar}, \quad (2.25)$$

where H is the time-independent Hamiltonian of the system. The time evolution of a pure state is governed by the Schrödinger equation, however, for a density operator this is described by the Von Neumann equation (also known as the Liouville–von Neumann equation) [74]:

$$\frac{d\rho(t)}{dt} = \frac{1}{i\hbar} [H, \rho(t)], \quad (2.26)$$

with the brackets denoting the commutation relation $[H, \rho] = H\rho - \rho H$. In the case that the Hamiltonian is time-dependent, for instance, if the system is subject to external parameters of control, we have that $H = H(t)$ in Eq. (2.26), and the time-evolution operator is given by the Dyson series [75]

$$\begin{aligned} U(t) &= \sum_{n=0}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n H(t_1) H(t_2) \cdots H(t_n) \\ &= \mathcal{T} \exp \left(-i \int_0^t H(t') dt' \right), \end{aligned} \quad (2.27)$$

where \mathcal{T} is the time-ordered operator, and we set $\hbar = 1$.

2.3.2 Quantum relative entropy

Now, we are going to discuss the quantum entropy and their basic properties. Moreover, the connection between the dissipation and fluctuations is established in the quantum mechanical world.

Von Neumann entropy

In this approach, the extension of the classical entropy to the quantum one is given by the von Neumann entropy [76],

$$S(\rho) := -\text{Tr}(\rho \ln \rho). \quad (2.28)$$

If we have a composite system such as ρ^{RS} , their partial states are given by

$$\rho^R := \text{Tr}_S(\rho^{RS}) \in \mathcal{B}(\mathcal{H}_R) \quad \text{and} \quad \rho^S := \text{Tr}_R(\rho^{RS}) \in \mathcal{B}(\mathcal{H}_S), \quad (2.29)$$

and their von Neumann entropies satisfy [77]

$$S(\rho^{RS}) \leq S(\rho^R) + S(\rho^S). \quad (2.30)$$

The equality is achieved only if $\rho^{RS} = \rho^R \otimes \rho^S$.

Quantum relative entropy and non-negativity

In the case we have two density matrices ρ and σ , the quantum relative entropy, also defined as the "distance" between them, is given by [78]

$$S(\rho||\sigma) := \text{Tr}(\rho \ln \rho) - \text{Tr}(\rho \ln \sigma). \quad (2.31)$$

If $\rho = \sigma$, the relative entropy is zero. Otherwise, if $\langle \psi | \rho | \psi \rangle \neq 0$ for any $|\psi\rangle$, and σ satisfies $\sigma | \psi \rangle = 0$, we have that $S(\rho||\sigma) = +\infty$. By considering two density operators written in terms of spectral decompositions,

$$\rho = \sum_a p(a) |\phi_a\rangle \langle \phi_a|, \quad (2.32)$$

$$\sigma = \sum_a q(a) |\phi_a\rangle \langle \phi_a|, \quad (2.33)$$

with the orthonormal basis $\{|\phi_a\rangle\}_{a \in \mathcal{A}}$, where $p(a)$ and $q(a)$ are probability distributions on a set \mathcal{A} , we get

$$S(\rho||\sigma) = S(p||q) \geq 0, \quad (2.34)$$

which is the classical relative entropy defined in (2.7). In this case, we can rewrite it in terms of discrete variables as

$$S(p||q) := \sum_a p(a) \ln \left(\frac{p(a)}{q(a)} \right). \quad (2.35)$$

The non-negativity in (2.34), also called the Klein's inequality, can be directly proved by using Jensen's inequality [41, 79] and it is essential to derive the second law.

2.3.3 Derivation of second law from the relative entropy

The starting point to obtain the QFT is to define which system we are analyzing and how its probability density is characterized. If we have a system interacting with a heat bath, for example, the Hamiltonian will be written as

$$H_{tot}(t) = H_S(t) + H_B + H_I(t). \quad (2.36)$$

Usually, we assume the weak coupling conditions, e. e. $\|H_S\| \gg \|H_I\|$ ³ and that the initial state of the system (S) and the bath (B) can be written in the product form

$$\rho_0^{SB} = \rho_S(0) \otimes \rho_B, \quad (2.37)$$

where

$$\rho_B = \frac{e^{-\beta H_B}}{Z} \quad (2.38)$$

stands for the thermodynamic equilibrium state in the canonical form while

$$Z = \text{Tr}(e^{-\beta H_B}), \quad (2.39)$$

is the partition function. $\beta = 1/T$ is the inverse temperature (Boltzmann constant is set to be one).

It is important to emphasize that the Gibbs distribution is a state that maximizes the entropy for a given energy, i.e., it is an equilibrium thermal state [80]. The final state of the composite system will be given by $\rho_t^{SB} = U \rho_0^{SB} U^\dagger$, where U is the unitary time-evolution operator given in (2.27).

Given the Von Neumann entropy in Eq. (2.28), the changes in this quantity will be then $\Delta S \equiv S(\rho_S(t)) - S(\rho_S(0))$. Also, the heat exchanged with the system can be written as

$$Q \equiv \text{Tr}[H_B(\rho_R - \rho_R(t))]. \quad (2.40)$$

³ $\|\cdot\|$ means the norm of the operator.

The Von Neumann entropy is invariant under unitary transformations, then $S(\rho_i) = S(\rho_f)$. Moreover, the total entropy production, denoted Σ , can be recast in the form [71]

$$\Sigma = S(\rho_t^{SB} || \rho_{ref}) \geq 0, \quad (2.41)$$

where ρ_{ref} is a reference equilibrium state that can be restated as $\rho_S(t) \otimes \rho'_B$. If $\rho_{ref} = \rho_t^{SB}$, the two distributions are equal and relative entropy is zero. Therefore, we can describe the total entropy production in the non-equilibrium dynamics of the composite system as

$$\Sigma \equiv \Delta S - \beta Q \geq 0. \quad (2.42)$$

The βQ term in this last expression can be understood as the entropy change in the bath [81]. Equation (2.42) is the second law of Thermodynamics in the form of the Clausius inequality, and it is a consequence of the non-negativity of the quantum relative entropy. Furthermore, it can be applied to arbitrary non-equilibrium states.

2.3.4 Stochastic Entropy Production

In order to formulate the QFT, we have to define the concepts of forward and reverse processes as trajectories in the state space, and establish stochastic thermodynamic quantities. Using the spectrum decomposition as in Eqs. (2.32) and (2.33), we can set two density operators, ρ_F and ρ_R , such as

$$\rho_F = \sum_a p_F(a) |\varphi_a\rangle \langle \varphi_a|, \quad (2.43)$$

$$\rho_R = \sum_b p_R(b) |\psi_b\rangle \langle \psi_b|, \quad (2.44)$$

where $\{|\varphi_a\rangle\}$ and $\{|\psi_b\rangle\}$ are orthonormal basis of \mathcal{H} . Here, the F and R labels means *forward* and *reverse* processes, respectively. In the following, we describe the protocols for both of these processes and also how to obtain the QFT from their probability distributions.

Forward Process

In the forward process, the initial state is given by ρ_F . If we perform a measurement on ρ_F in the basis $\{|\varphi_a\rangle\}$, we will have an outcome a with probability $p_F(a) = \text{Tr}[\Pi_a \rho_F]$, with $\Pi_a = |\varphi_a\rangle \langle \varphi_a|$ is the projector. The final state ρ_{F_f} is then given by

$$\rho_{F_f} = U \Pi_a \rho_F \Pi_a U^\dagger / p_F(a), \quad (2.45)$$

where U is the evolution operator representing the process under consideration. If we perform another measurement on this new state, but now in basis $\{|\psi_b\rangle\}$, we obtain an outcome b with probability $p_{F_f}(b) = \langle\psi_b|\rho_{F_f}|\psi_b\rangle$. Thus, we can define a transition probability, $p(a \rightarrow b)$, that is the probability of moving from one state to another during a single realization of the process, as

$$p(a \rightarrow b) = \text{Tr}[\Pi_b U \rho_{F_f} U^\dagger]. \quad (2.46)$$

From this result, we can calculate the joint probability of the outcomes (a, b) as

$$p(a, b) = p_F(a) p(a \rightarrow b), \quad (2.47)$$

and also, $\sum_a p(a, b) = p_{F_f}(b)$.

Reverse Process

In the reverse process, we can construct a similar protocol, but with some changes. Here, we have to pay attention in the action of a *time-reversal operator* on the initial state ρ_R and on the Hamiltonian. First, we note that ρ_R , the density operator that describe the initial state in the reverse process, is given by

$$\tilde{\rho}_R = \sum_b p_R(b) |\tilde{\psi}_b\rangle \langle\tilde{\psi}_b| := \Theta \rho_R \Theta, \quad (2.48)$$

where Θ is the time-reversal operator, an anti-unitary operator satisfying $\Theta^2 = \Theta$ and $\Theta^\dagger = \Theta$, and $\Theta |\psi_b\rangle := |\tilde{\psi}_b\rangle$.

The reverse protocol is the following. If we perform a measurement on $\tilde{\rho}_R$ in basis $\{|\tilde{\psi}_b\rangle\}$, we obtain an outcome b with probability $p_R(b) = \text{Tr}[\tilde{\Pi}_b \tilde{\rho}_R]$. Next, we evaluate the time evolution from $t = 0$ to $t = \tau$, by using the corresponding unitary operator \tilde{U} , defined here as

$$\tilde{U} = T \exp \left(-i \int_0^\tau \tilde{H}(\tau - t) dt \right), \quad (2.49)$$

where $\tilde{H}(t) := \Theta H(t) \Theta$ is the time-reversed Hamiltonian. Then, if we perform another measurement in the state $\tilde{U} \tilde{\rho}_R \tilde{U}^\dagger$, which gives the reverse state after applying the unitary evolution operator during a certain time, but now in basis $\{|\tilde{\varphi}_a\rangle\}$, we obtain the outcome a with probability $\tilde{p}_{R_f}(a) = \text{Tr}[\tilde{\Pi}_a \tilde{U} \tilde{\Pi}_b \tilde{\rho}_R \tilde{\Pi}_b \tilde{U}^\dagger] / p_R(b)$.

Thus, we can also define a reverse transition probability, $\tilde{p}(b \rightarrow a)$ as

$$\tilde{p}(b \rightarrow a) = \text{Tr}[\tilde{\Pi}_a \tilde{U} \tilde{\Pi}_b \tilde{\rho}_R \tilde{\Pi}_b \tilde{U}^\dagger]. \quad (2.50)$$

From this result, we can calculate the joint probability of the outcomes (a, b) in the reverse process as

$$\tilde{p}(b, a) = p_R(b) \tilde{p}(b \rightarrow a), \quad (2.51)$$

and also, $\sum_b \tilde{p}(b, a) = \tilde{p}_{R_f}(a)$.

Average Entropy Production

After describing the protocols for the forward and reverse processes, one can define the *stochastic entropy production* for both in the following way [79]

$$\sigma(a, b) := \ln \frac{p(a, b)}{\tilde{p}(b, a)} \quad (\text{forward process}), \quad (2.52)$$

$$\tilde{\sigma}(b, a) := \ln \frac{\tilde{p}(b, a)}{p(a, b)} \quad (\text{reverse process}), \quad (2.53)$$

where we have applied the fluctuation theorems seen before in the first section of this Chapter. One can note that $\sigma(a, b) = -\tilde{\sigma}(b, a)$. Moreover, this last equations directly lead to a general expression of the quantum fluctuation theorem. The average of σ in the forward process is given by [68]

$$\langle \sigma \rangle = \sum_{a,b} p(a, b) \ln \frac{p(a, b)}{\tilde{p}(b, a)} \geq 0. \quad (2.54)$$

This last expression is just the quantum relative entropy in (2.35). Now, let us introduce the following probabilities distributions of σ and $\tilde{\sigma}$:

$$p(\sigma = \Sigma) := \sum_{a,b} p(a, b) \delta(\sigma, \Sigma), \quad (2.55)$$

$$\tilde{p}(\tilde{\sigma} = -\Sigma) := \sum_{a,b} \tilde{p}(b, a) \delta(\tilde{\sigma}, -\Sigma). \quad (2.56)$$

Here, δ is the Kronecker delta and $\delta(\tilde{\sigma}, -\Sigma) = \delta(\sigma, \Sigma)$. We can therefore show that

$$\begin{aligned} \tilde{p}(\tilde{\sigma} = -\Sigma) &= \sum_{a,b} p(a, b) e^{\tilde{\sigma}(a,b)} \delta(\tilde{\sigma}, -\Sigma) \\ &= e^{-\Sigma} \sum_{a,b} p(a, b) \delta(\tilde{\sigma}, -\Sigma) \\ &= e^{-\Sigma} p(\sigma = \Sigma) \end{aligned}$$

Therefore, we can finally obtain the quantum fluctuation theorem in the form

$$\frac{\tilde{p}(\tilde{\sigma} = -\Sigma)}{p(\sigma = \Sigma)} = e^{-\Sigma}. \quad (2.57)$$

From this result, we can also show that $\langle e^{-\Sigma} \rangle = 1$, which is the integral fluctuation theorem, or quantum Jarzynski equality [82].

2.4 Beyond the second law: Uncertainty Relations

In addition to the second law of thermodynamics, which says that entropy production must always be non-negative, we will show that the entropy production has a minimum value, and this value is greater than zero for irreversible processes. Furthermore, we can show that this lower bound play a major role in controlling variances.

2.4.1 Classical Thermodynamic Uncertainty Relations

Minimal cost of precision

To understand how we derive a TUR, let us take as example a stochastic process in a biological context, which is the focus of the article by Udo Seifert and Andre Barato [14]. Here, the process in which chemical reactions catalyzed by enzymatic cycles converts chemical free energy from adenosine triphosphate molecule (ATP) into mechanical work is outlined. This is what is called a molecular engine, and in this case, the observable of interest is the number of steps the engine takes, and such as any stochastic variable, it is subject to thermal fluctuations.

Considering a linear network of states of a chemical reaction out of equilibrium catalyzed by an enzyme, the observable in question, or the output is given by completion of an enzymatic cycle that forms a single step, $X(t)$. Such steps occur at a rate k^+ or k^- , with k^+ in one direction and k^- in the opposite direction, as shown in Fig. 2.3. Then, after a time t , we will have an average of $\langle X \rangle = (k^+ - k^-)t = Jt$ steps, where J is the probability current, also called "speed" in the steady-state.

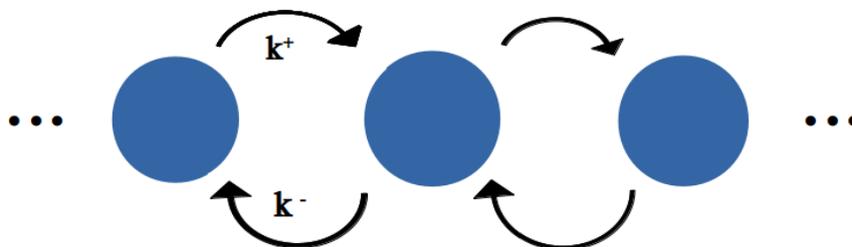


FIGURE 2.3: Linear network of states of a chemical reaction.

If we calculate the variance of several realizations of this random process, we obtain [36]

$$\text{Var}(X) = \langle (X - \langle X \rangle)^2 \rangle = (k^+ + k^-)t = 2Dt, \quad (2.58)$$

where D is the diffusion coefficient. Therefore, with the mean and the variance we get the squared relative uncertainty of the observable in terms of current and diffusion:

$$\varepsilon^2 \equiv \frac{\text{Var}(X)}{\langle X \rangle^2} = \frac{2D}{J^2 t}. \quad (2.59)$$

In order to obtain the thermodynamic cost C generated by the output, which in a period t is given by the entropy production rate σ , we have

$$C = \sigma t = (k^+ - k^-) \ln \left(\frac{k^+}{k^-} \right) t. \quad (2.60)$$

In this last expression, one can assume an external environment at a fixed temperature T where the transition rates are given by the local detailed balance (LDB) relation [83],

$$\frac{k^+}{k^-} = \exp(\mathcal{A}/k_B T), \quad (2.61)$$

which describes an equilibrium relationship between opposite processes and comes from the fluctuation theorems discussed in the earlier sections. Here, \mathcal{A} is the affinity driving the process, associated with the variable X . In this case, for instance, when X is a number associated to a chemical reaction, \mathcal{A} can be the chemical potential difference, $\mathcal{A} = \mu_{ATP} - \mu_{ADP} - \mu_P$.

Therefore, we see that the relationship between thermodynamic cost and uncertainty, or in other words, the energy dissipated in the process and precision, is given by the following thermodynamic uncertainty relation

$$C\varepsilon^2 = 2\sigma D/J^2 \geq 2k_B T, \quad (2.62)$$

where σ is the rate of entropy production, and this minimum limit of $2k_B T$ is independent of time. Furthermore, if we isolate σ , we find that the entropy production has the minimum value of $(J^2/D)k_B T$. This shows that to obtain a maximum or perfect precision, which would be a zero uncertainty, we would have infinite energy, which is impossible. Therefore, there is a *minimal cost of precision* that is unavoidable and universal in any process of this type. Note that the same results were earlier obtained, using a distinct method, in Ref. [1], which holds for both classical and quantum systems.

Uncertainty bound on variance of current fluctuations

A generalization of the TUR obtained before is given in an article by Gingrich *et al.* of 2016 [15], which demonstrates that in a context of non-equilibrium steady-states, all the current fluctuations are subject to a bound in the trade-off relation between the energy cost and the precision of measurement. In this work, the thermodynamic uncertainty relation is given by

$$\epsilon^2 \Sigma^\pi \geq 2, \quad (2.63)$$

where ϵ^2 is the relative uncertainty of current fluctuations

$$\epsilon^2 = \frac{\text{Var}(j)}{\langle j^\pi \rangle^2}. \quad (2.64)$$

It is the variance normalized by the mean of a generalized current j , and the index π refers to steady-state. Also, Σ^π is the average dissipation rate, and Boltzmann's constant and the temperature was set as equal to 1.

Equation (2.63) means that when the relation between the dissipation and the uncertainty of the generalized current is calculated, it is verified that this value must be greater than or equal to 2. That is, controlling the current fluctuations by reducing the relative uncertainty costs a minimum dissipation. For example, if we want a precision of 1%, this costs at least $20.000k_B T$. This is an inevitable cost of temporal precision considering a stationary Markov process (i.e., a stochastic process that satisfies the "memoryless" property [84]).

2.4.2 Quantum thermodynamic uncertainty relations

In the quantum regime, the classical TUR described in the expressions (2.62) and (2.63) can be violated [85, 25], and it is still not entirely known why this happens. In fact, this is an interesting topic of research in the recent years, for instance, in the development of nanoscale autonomous machines that operate in non-equilibrium conditions [86]. Recently, it has been shown [16] that, for non-equilibrium quantum steady-states (NESS), the thermodynamic uncertainty relation is described as a direct consequence of the Cramér-Rao bound (CRB), and the geometry of quantum NESS itself directly implies the existence of a TUR in the form

$$\frac{\Delta_J}{\langle J \rangle^2} \langle \sigma \rangle \geq 1, \quad (2.65)$$

where J is the current—that can be of heat, charge or particles—, $\langle J \rangle$ is the average over all the currents, and Δ_J is the normalized variance,

$$\Delta_J \equiv \lim_{\tau \rightarrow \infty} \tau (\langle J^2 \rangle - \langle J \rangle^2). \quad (2.66)$$

Also, $\langle \sigma \rangle$ is defined as the average entropy production rate in the NESS. Equation (2.65) states a fundamental limit for precision thermodynamics for the NESS, which is twice smaller than that found in the classical regime. In the following, we will briefly derive the quantum TUR. The explicit derivation is found in more details in the reference [16]. See also Ref. [1] for a similar derivation.

Proof of the TUR in (2.65)

The main idea behind this approach is to exploit the mathematical properties of the quantum relative entropy between two probability densities and relate this to the entropy production in the context of non-equilibrium steady-states (NESS). After performing some calculations and transformations, the quantum TUR is obtained. For the case considered, the typical NESS scenario is described in Fig. 2.4, by which a quantum system is connected to two reservoirs (L, for "left", and R, for "right") that drive the system into a global steady-state. Then, a density matrix ensemble description is used in order to characterize observables that are directly connected with the entropy production and current fluctuations.

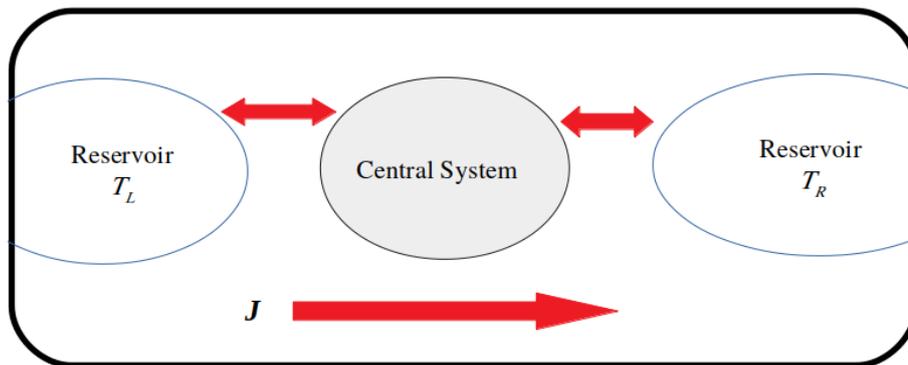


FIGURE 2.4: Diagrammatic illustration of a central system coupled to two thermal reservoirs at temperatures $T_{L,R}$. After a long time, this system will tend to a global non-equilibrium steady-state (NESS) characterized by a current J (of particles, charge, heat, etc...).

First, let us define the geometry of the states for the problem at hand. Here, we are going to consider a *manifold of steady-states* (SSM) (see Fig. 2.5), where the relation between two steady-states is quantified by their distinguishability measure through the relative entropy (Kullback-Leibler divergence) given in Eq. (2.31). Then,

we can rewrite this as

$$D(\rho_1||\rho_2) = \text{Tr}[\rho_1 \ln \rho_1] - \text{Tr}[\rho_1 \ln \rho_2]. \quad (2.67)$$



FIGURE 2.5: Manifold of non-equilibrium steady-states and the relative entropy between two density operators.

However, for the system considered here, the density matrices will correspond to $\rho_1 \rightarrow \rho_{ness}$ and $\rho_2 \rightarrow \rho_{les}$, where this last one representing the *local equilibrium state* (LES) of the total system. It means that the equilibrium condition is reached when both reservoirs have the same inverse temperature and chemical potential.

The time evolution of the entire composite system from the infinite past to the present is obtained through a generalized Gibbs ensemble, also known as the McLennan-Zubarev form [87, 88, 89, 90, 91]. Therefore, we can write the NESS and LES density matrices as

$$\rho_{ness} = \frac{e^{-\bar{\beta}(\mathcal{H} - \bar{\mu}N) + \Sigma}}{Z_{ness}}, \quad \rho_{les} = \frac{e^{-\bar{\beta}(\mathcal{H} - \bar{\mu}N)}}{Z_{les}}, \quad (2.68)$$

where Z represents the partition function, $\bar{\beta} = (\beta_L + \beta_R)/2$ is the average of the inverse temperatures, $\bar{\mu} = (\beta_L \mu_L + \beta_R \mu_R)/(\beta_L + \beta_R)$ is the mean chemical potential, $N \equiv \sum_{a=L,R} N_a$ is the total particle number, \mathcal{H} is the total Hamiltonian and Σ is the *entropy production* that is defined as

$$\Sigma = \delta_{\mu\beta} Q - \delta_{\beta} E, \quad (2.69)$$

where $E = (\mathcal{H}_L - \mathcal{H}_R)/2$, $Q = (N_L - N_R)/2$, are the time-average energy and particle difference between L and R , and $\delta_{\mu\beta} = \mu_L \beta_L - \mu_R \beta_R$, $\delta_{\beta} = \beta_L - \beta_R$ are known as thermodynamic affinities that drive the particle and energy currents, respectively [92].

From the relation in Eq. (2.69), we can define the *average entropy production rate* in the usual form as

$$\langle \sigma \rangle = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \langle \Sigma \rangle = \delta_{\mu\beta} \langle J_Q \rangle - \delta_{\beta} \langle J_E \rangle, \quad (2.70)$$

where $J_{Q,E}$ are the particle and energy currents in the SSM, defined as

$$J_Q(t) \equiv \frac{dQ(t)}{dt}, \quad J_E(t) \equiv \frac{dE(t)}{dt}, \quad (2.71)$$

and the time-averaged currents in the NESS are given by $\langle J_{Q,E} \rangle = \text{Tr}[J_{Q,E} \rho_{ness}]$. If we explicit calculate the the relative entropy between ρ_{ness} and ρ_{les} , we will get that

$$\begin{aligned} D(\rho_{ness}||\rho_{les}) &= \text{Tr} \left[\rho_{ness} \ln \left(\frac{\rho_{ness}}{\rho_{les}} \right) \right] \\ &= \text{Tr} \left[\rho_{ness} \ln \left(e^\Sigma \frac{Z_{les}}{Z_{ness}} \right) \right] \\ &= \text{Tr} \left[\rho_{ness} \left(\Sigma - \ln \left(\frac{Z_{ness}}{Z_{les}} \right) \right) \right] \\ \therefore D(\rho_{ness}||\rho_{les}) &= \langle \Sigma \rangle - \ln \left(\frac{Z_{ness}}{Z_{les}} \right). \end{aligned} \quad (2.72)$$

Here, we used the trace properties: $\text{Tr}[\rho_{ness} \Sigma] = \langle \Sigma \rangle$ and $\text{Tr}[\rho_{ness}] = 1$. The last term in Eq. (2.72) can be interpreted as the difference between thermodynamic potentials in the LES and NESS, denoted as ψ_{les} and ψ_{ness} , also called Massieu functions [93]. Also, because the time-averaged entropy production Σ is a conserved quantity and commutes with \mathcal{H} and N , we can use the exponential matrix property $e^{A+B} = e^A e^B$ and rewrite the last term as

$$\begin{aligned} \Delta\psi &= \psi_{les} - \psi_{ness} = \ln \left(\frac{Z_{ness}}{Z_{les}} \right) = \ln \left(\frac{\text{Tr}[e^{-\bar{\beta}(\mathcal{H}-\bar{\mu}N)} e^\Sigma]}{\text{Tr}[(e^{-\bar{\beta}(\mathcal{H}-\bar{\mu}N)})]} \right) \\ &= \ln \left(\text{Tr} \left[\frac{e^{-\bar{\beta}(\mathcal{H}-\bar{\mu}N)}}{\text{Tr}[(e^{-\bar{\beta}(\mathcal{H}-\bar{\mu}N)})]} e^\Sigma \right] \right) = \ln(\text{Tr}[\rho_{les} e^\Sigma]). \end{aligned} \quad (2.73)$$

Now, we can expand the exponential in Taylor series about zero, also called Maclaurin series,

$$e^\Sigma = \sum_{k=0}^{+\infty} \frac{\Sigma^k}{k!}, \quad (2.74)$$

whereby gives us

$$\begin{aligned} \Delta\psi &= \ln \left(1 + \sum_{n=0}^{+\infty} \text{Tr} \left[\rho_{les} \left(\frac{\Sigma^{(2n+1)}}{(2n+1)!} \right) \right] + \text{Tr} \left[\rho_{les} \left(\sum_{n=1}^{+\infty} \frac{\Sigma^{(2n)}}{(2n)!} \right) \right] \right) \\ &= \ln \left(1 + \sum_{n=1}^{+\infty} \frac{\langle \Sigma^{(2n)} \rangle_{les}}{(2n)!} \right). \end{aligned} \quad (2.75)$$

The first term comes from $k = 0$ in Eq. (2.74), which gives that $\text{Tr}[\rho_{les}] = 1$. The

others terms in the expansion were assembled into even and odd powers of the entropy production. Then, because the expectation value is taken over ρ_{les} , the odd terms vanish.

Now, we are going to perform a transformation in the SSM, by rewriting the NESS density matrix as a generalized function of the control parameter λ ,

$$\rho_{ness} \equiv \rho(\lambda),$$

where $\lambda = (\bar{\beta}, \bar{\beta}\mu, \delta_\beta, \delta_{\beta\mu})^T$ can be described as the vector of the parameters that define the thermodynamic conditions in the SSM. If the system is subject to small variations on the control parameter λ , $\rho(\lambda) \mapsto \rho(\lambda + \delta\lambda)$, and then the relative entropy between these two states can be given by the local curvature of the manifold. This can be calculated in terms of the *Fisher Information* (I) as [94, 95]

$$D(\rho(\lambda + \delta\lambda) || \rho(\lambda)) = \frac{1}{2} d\lambda^T I(\lambda) d\lambda + O(d\lambda^3), \quad (2.76)$$

where I quantifies the sensitivity of the system when small variations of λ are made, and it is defined in the multidimensional case as a matrix whose elements are written as

$$I(\lambda)_{ij} = \sum_k \rho_k(\lambda) \left(\frac{\partial \ln \rho_k(\lambda)}{\partial \lambda_i} \frac{\partial \ln \rho_k(\lambda)}{\partial \lambda_j} \right). \quad (2.77)$$

The precision of estimation of a parameter λ , or a function $f(\lambda)$, is determined by a fundamental lower bound, called *Cramér-Rao bound* (CRB) [41, 96], that can be written in terms of Fisher information in this case as

$$\text{Cov}_\lambda(f) \geq \frac{\partial f(\lambda)}{\partial \lambda} [I(\lambda)]^{-1} \left(\frac{\partial f(\lambda)}{\partial \lambda} \right)^T, \quad (2.78)$$

where $\text{Cov}_\lambda(f)$ is the covariance matrix of $f(\lambda)$, and its elements are given by $\text{Cov}_\lambda(f_i f_j) = \langle f_i f_j \rangle_\lambda - \langle f_i \rangle_\lambda \langle f_j \rangle_\lambda$. The partial derivative of $f(\lambda)$ with respect to λ is the Jacobian matrix whose ij element is given by $\partial f_i(\lambda) / \partial \lambda_j$. We can use the CRB to estimate the average steady-state currents $\langle J_\alpha \rangle_\lambda$, where the α label can be any current defined in the system. Let us define

$$K_\lambda(J) \equiv \frac{d \langle J \rangle}{d\lambda} \quad (2.79)$$

as the Jacobian matrix and

$$\text{Cov}_\lambda(J_\alpha, J_{\alpha'}) = \text{Tr}[J_\alpha J_{\alpha'} \rho(\lambda)] - \text{Tr}[J_\alpha \rho(\lambda)] \text{Tr}[J_{\alpha'} \rho(\lambda)] \quad (2.80)$$

as the covariance matrix $\text{Cov}_\lambda(J)$. Then, the CRB can be written as

$$\text{Cov}_\lambda(J) - K_\lambda(J) [I(\lambda)]^{-1} (K_\lambda(J))^T \geq 0. \quad (2.81)$$

This last expression can also be rewritten as $I - K^T \text{Cov}^{-1} K \geq 0$ [97]. From the expression in Eq. (2.79), we can write $d\langle J \rangle = K d\lambda$, what allows us to express the inequality in question as

$$d\lambda^T I d\lambda \geq d\langle J \rangle^T \text{Cov}^{-1} d\langle J \rangle \quad (2.82)$$

$$2D(\rho_{ness} || \rho_{les}) \geq \langle J \rangle^T \text{Cov}^{-1} \langle J \rangle \quad (2.83)$$

$$(\langle \Sigma \rangle - \Delta\psi) \geq \frac{1}{2} \langle J \rangle^T \text{Cov}^{-1} \langle J \rangle. \quad (2.84)$$

From Eq. (2.82) to (2.83), we have used the relation in Eq. (2.76), where we can consider the NESS and LES states in terms of the control parameter λ , and also $d\langle J \rangle = \langle J \rangle_{ness} - \langle J \rangle_{les} = \langle J \rangle_{ness} \equiv \langle J \rangle$, since the currents are zero in the LES. From Eqs. (2.83) to (2.84) we have substituted the relative entropy relation in Eq. (2.72).

Now, we can notice that from Eq. (2.75), we have that $\Delta\psi = \langle \Sigma^2 \rangle_{les} / 2 + O^3$. However, by following the calculations detailed in Ref. [16], where the expansion in the relation between the partition functions in the NESS and LES leads to the relation $\langle \Sigma^2 \rangle_{les} + O^3 = \langle \Sigma \rangle_{ness}$, i.e., the average of the squared entropy production in the LES is equal, up to the second order, to the average entropy production in the NESS. Thus, we can finally write that in the regime of small temperatures,

$$\Delta\psi = \frac{\langle \Sigma^2 \rangle_{les}}{2} + O^3 = \frac{\langle \Sigma \rangle_{ness}}{2}. \quad (2.85)$$

Therefore, the inequality in Eq. (2.84), by considering $\langle \Sigma \rangle = \langle \Sigma \rangle_{ness}$, will be given by

$$\langle \Sigma \rangle \geq \langle J \rangle^T \text{Cov}^{-1} \langle J \rangle. \quad (2.86)$$

This last result can be expressed in terms of the average steady-state entropy production rate in Eq. (2.70),

$$\langle \Sigma \rangle = \lim_{\tau \rightarrow \infty} \tau \langle \sigma \rangle, \quad (2.87)$$

and with the normalized covariance matrix between different steady-states currents [98],

$$\Delta(J_\alpha J_{\alpha'}) = \lim_{\tau \rightarrow \infty} \tau \text{Cov}(J_\alpha J_{\alpha'}), \quad (2.88)$$

and we can finally obtain a TUR in the form

$$\frac{\Delta_J}{\langle J \rangle^2} \langle \sigma \rangle \geq 1, \quad (2.89)$$

where we have considered $\langle J \rangle$ a symmetric matrix, and then $\langle J \rangle = \langle J \rangle^T$. Equation (2.89), when compared to its classical counterpart, shows that the bound on the variance of the currents can be at least twice smaller. This kind of violation of the TUR is interesting because this trade-off relation can be linked to power fluctuations of a heat engine, and consequently, to its stability and efficiency, what it is essential in the development of a range of measurement devices. A similar approach in the context of a general estimation process is given in Ref. [1], where it is introduced a bound on the precision of acquiring information in terms of dissipated work, and it has practical applications such as increase efficiency of the reversibility of high precision measurement devices in metrology. Recently, the violation of the TUR was analyzed in the context of quantum thermoelectric junctions at steady state [85], to quantify the performance of thermoelectric generators, i.e, its power fluctuations efficiency.

Chapter 3

Quantum Mechanics in Phase Space

WHAT is phase space? When we think about the environment that surrounds us, we notice that it has characteristics such as size, colors, sounds, temperature, etc ... What we see, in fact, always has width, length, and depth, and so our displacement is subject to such bonds with the space we step on. In the classical world, we have named such characteristics as the dimensions x , y , z . So, classical space (from our direct experience) is a Cartesian representation of Euclidean geometry [99]. However, there is another way to describe the space in question, using parameters other than just x , y , z .

If, for instance, we want to know how a body moves in this space, we need to know its speed and where it was. In turn, velocity is a measure of displacement for a certain time, and if we make the product of this variation of space in time by the mass of the body, we obtain its generalized linear momentum. With the momentum, we can describe the trajectory of the body in motion, but to know how it changes its speed in space being traversed, we need another form of representation, different from the Cartesian graphs before. We need to describe a phase space, where one can see how the state of the body changes. This is what phase space represents: all possible states of the dynamics of a system [21].

3.1 Classical mechanics

Classically, the points defined in this space are pairs of parameters (also known as degrees of freedom or generalized coordinates) \mathbf{p} and \mathbf{q} , momentum, and position, respectively. Each point represents a state of the system, and each parameter is represented by an axis of a multidimensional space. The Hamiltonian of the system of interest is a function of both generalized coordinates and time, $H(\mathbf{q}, \mathbf{p}, t)$ and it fully describes the mechanics of the system. If we analyze the generalized coordinate \mathbf{q} with respect to time, we get information about the *trajectory* of the system, but we have no information about its *motion*. On the contrary, if we analyze the generalized conjugate moment \mathbf{p} concerning time, we have the *temporal evolution*

of the momentum, and consequently, the *energy* of the system. However, we do not have the trajectory. On the other hand, the analysis of \mathbf{p} with \mathbf{q} allows us to examine the evolution of both coordinates without explicitly dependence on time. For instance, in the case of a system that oscillates periodically, or a *harmonic oscillator*, subject to a potential $U(x) \propto x^2/2$, we can schematize the evolution of the states variables, x (which gives the displacement) and p (which gives the momentum), as shown in Fig. 3.1, and the trajectory in the phase space related to the action of this system (Fig. 3.2).

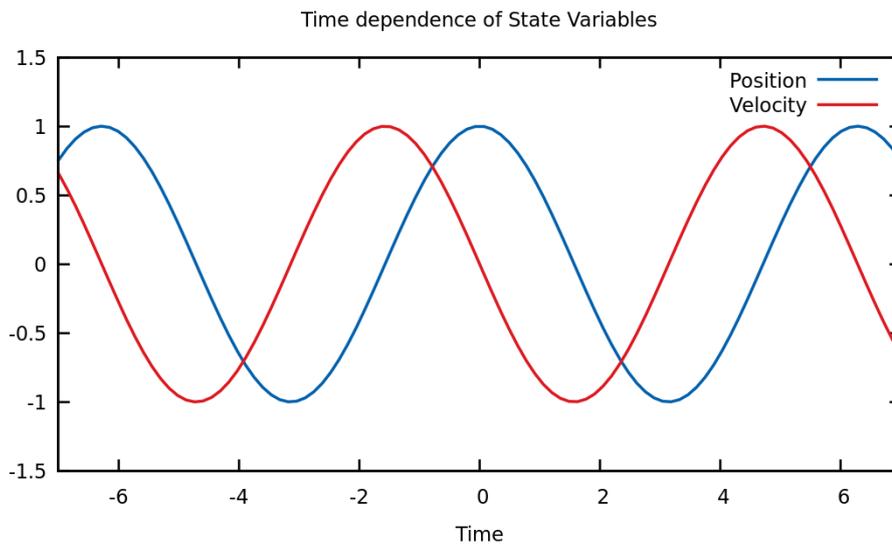


FIGURE 3.1: Time evolution of a simple harmonic oscillator.

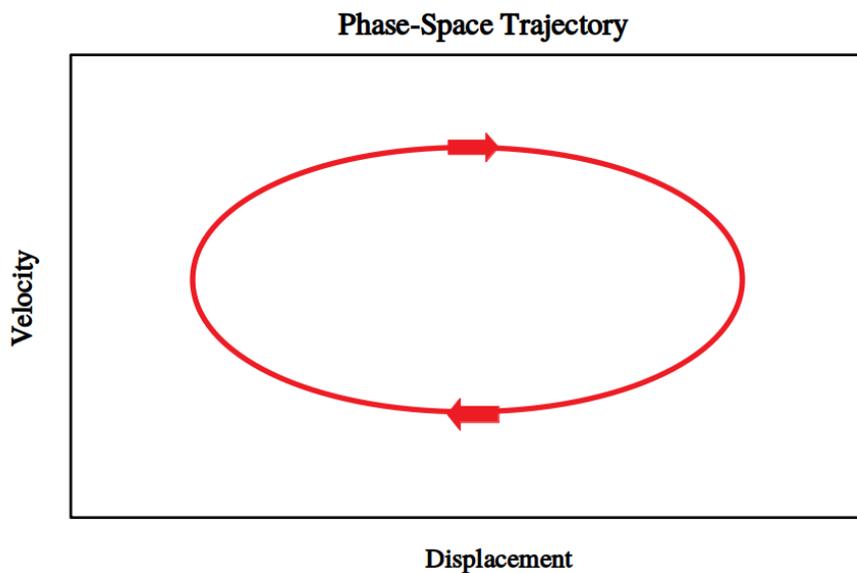


FIGURE 3.2: Illustration of a trajectory in phase space for a simple harmonic oscillator.

The analysis of \mathbf{p} with respect to \mathbf{q} is the *phase space dynamics*, and it allows us to express the Hamiltonian or the system's equations of motion in terms of \mathbf{p} and \mathbf{q} only, as described by Hamilton's equations [21]

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}. \quad (3.1)$$

3.1.1 Hamiltonian flow and continuity equation

The initial conditions defined by a point in phase space lead to the description of individual trajectories and Hamilton's equations that guide the evolution of the system of interest. In the case of a system subject to a flow of a Hamiltonian function, Hamilton's equations can be written in a matrix notation as [100]

$$\begin{pmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{pmatrix} = \mathbf{M}_2 \begin{pmatrix} \frac{\partial H}{\partial \mathbf{q}} \\ \frac{\partial H}{\partial \mathbf{p}} \end{pmatrix}, \quad (3.2)$$

where \mathbf{M}_2 is the standard symplectic matrix of order 2 given by

$$\mathbf{M}_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The general dynamics of a function $F(q_i, p_i; t)$, where q_i and p_i are, respectively, the canonical coordinates and conjugate momenta ($i = 1, \dots, n$), can be written as a *continuity equation* that, more generally, may include a "source" and a "sink" term, also functions of q_i , p_i , and t , when we want to describe quantities that are often but not always conserved

$$\frac{\partial F}{\partial t} + \nabla \cdot \mathbf{J} = \sigma, \quad (3.3)$$

where $\nabla = (\frac{\partial}{\partial q_i}, \frac{\partial}{\partial p_i})$, and \mathbf{J} represents the phase space current while σ is the generating source or sink contributions.

If the system is conservative, then $\sigma = 0$ and the total time derivative of the function F is also zero. Therefore, the continuity equation can be written as a Liouville equation [101], since

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \sum_{i=1}^n \left(\frac{\partial F}{\partial q_i} \dot{q}_i + \frac{\partial F}{\partial p_i} \dot{p}_i \right) = 0, \quad (3.4)$$

or, by relating the terms in the sum with the derivatives in Eq. (3.1),

$$\frac{\partial F}{\partial t} + \{F, H\} = 0, \quad (3.5)$$

where

$$\{F, H\} = \sum_{i=1}^n \left(\frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \quad (3.6)$$

is the Poisson bracket. For the canonical coordinates, we have

$$\{q_i, q_j\} = \{p_i, p_j\} = 0 \quad (3.7)$$

$$\{q_i, p_j\} = \delta_{ij} \quad , \quad (3.8)$$

where δ_{ij} is the Kronecker delta.

Comparing Eqs. (3.3) and (3.5), we see that $\nabla \cdot \mathbf{J} = \{F, H\}$, and then the classical current in phase space can be written as

$$\mathbf{J} = \begin{pmatrix} J_q \\ J_p \end{pmatrix} = \begin{pmatrix} \dot{q}^F \\ \dot{p}^F \end{pmatrix} \quad (3.9)$$

3.2 Quantum mechanics

In classical mechanics, we can structure a map that relates the generalized coordinates and the conjugate momenta and study how they evolve, in the same perspective, through a phase space distribution, $\rho(q, p)$, which determines the probability that the system will be found in a given microstate $(q + dq, p + dp)$, with a infinitesimal probability element $\rho dp dq$. In quantum mechanics, however, the Heisenberg uncertainty relation tells us that we cannot precisely define these two variables at the same time with infinity precision [18]. Representations of states in quantum mechanics are made in terms of either position or momentum, but not both.

The dynamics of a quantum system are subject to parameter fluctuations, which makes the definition of a trajectory somewhat more uncertain. Because of this statistical nature, the state of the system, which in the formulation in Hilbert space is described by a state vector or wave function, is represented in phase space as a *quasiprobability* distribution.

In the 20th century, several people studied the formulation of quantum mechanics in the phase space based on this concept of a quasiprobability distribution. One of the first was the physicist Eugene Wigner, winner of the 1963 Nobel Prize in Physics "for his contributions to the theory of the atomic nucleus and the elementary particles, particularly through the discovery and application of fundamental symmetry principles" [102]. The Wigner function¹ is one of the pillars of the formulation of quantum mechanics in phase space, although there are others. It was introduced in 1932 to study quantum corrections to classical statistical mechanics [103]. In

¹See Appendix C.

1927 Hermann Weyl introduced the concept of mapping from phase space functions to Hilbert space operators in the Schrödinger picture, also known as Weyl transform or Weyl quantization [104]. The inverse mapping is called Wigner transform. Later, this inversion of representations was very useful in the works carried out by Hilbrand J. Groenewold [105] in 1946, and José Enrique Moya in 1949 [106].

To understand how we relate the classical and quantum representations, we need to construct a basis where we can develop the main conceptions we are dealing with. This framework is based on the problems of systems that are nearly classical but have some important quantum features. It is often faced in quantum optics, where characterizing fluctuating classical fields is necessary [107]. In this context, we will see that the formalism based on the study of coherent states of oscillating radiation fields is a very useful way to describe the dynamics in phase space.

3.2.1 The Harmonic Oscillator

One of the best examples of quantum systems in which we can study certain classical properties is the harmonic oscillator. In the classical description, a particle of mass m in an oscillatory motion can be described by its position and momentum, both of which changing in time. The total energy of this system is given by

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2, \quad (3.10)$$

where ω is the angular frequency and it is related to the period of oscillation T by $\omega = 2\pi/T$. The harmonic oscillator can also appear when analyzing the one-dimensional oscillations in a spring of elastic constant k , subject to a restoring force of the form $F = -kx$. In this case, the angular frequency is defined as $\omega = \sqrt{k/m}$.

To define the quantum system, we have to change concepts. Now, let us use Hermitian operators in place of dynamic variables, which follow the commutation relations

$$[q, p] = i\hbar. \quad (3.11)$$

In the following step, one can define a Hamiltonian for this *quantum* harmonic oscillator as

$$H \equiv \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2. \quad (3.12)$$

Creation and annihilation operators

For the convenience of a better description of the problem, we can define two non-Hermitian operators, called *annihilation* and *creation* operators [72], respectively,

such that

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(q + \frac{ip}{m\omega} \right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(q - \frac{ip}{m\omega} \right). \quad (3.13)$$

From the canonical commutation relations, one can obtain directly that

$$[a, a^\dagger] = 1. \quad (3.14)$$

Definition 3. We define a **number operator**, or **occupation number operator**, as

$$N = a^\dagger a,$$

which is clearly Hermitian. Also, a direct calculation leads to

$$a^\dagger a = \frac{H}{\hbar\omega} - \frac{1}{2}.$$

Therefore, one can rewrite the Hamiltonian operator in Eq. (3.12) for the quantum harmonic oscillator as

$$H = \hbar\omega \left(N + \frac{1}{2} \right) = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right). \quad (3.15)$$

Since the Hamiltonian and the number operator commutes with each other, they share a set of joint eigenstates denoted by

$$N |n\rangle = n |n\rangle, \quad (3.16)$$

and

$$H |n\rangle = E_n |n\rangle, \quad (3.17)$$

where $|n\rangle$ are known as energy eigenstates. Due to Eq. (3.15), we also have

$$H |n\rangle = \left(n + \frac{1}{2} \right) \hbar\omega |n\rangle, \quad (3.18)$$

what leads to the energy eigenvalues given by

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega. \quad (3.19)$$

Now, we seek to better characterize this eigenstate of the number operator, $|n\rangle$. What would be the eigenvalues and eigenvectors of N ?

Let us begin by considering that, since N is Hermitian, its eigenvalues must be real and its eigenvectors form an orthonormal basis. From the definition of H in

terms of $a^\dagger a$ and Eq. (3.16), we can write

$$a^\dagger a |n\rangle = n |n\rangle, \quad (3.20)$$

from which we obtain

$$\langle n | a^\dagger a |n\rangle = n \geq 0. \quad (3.21)$$

Using the relation in Eq. (3.14) along with $[AB, C] = A[B, C] + [A, C]B$, one can show that

$$[a^\dagger a, a] = -a, \quad [a^\dagger a, a^\dagger] = a^\dagger. \quad (3.22)$$

Therefore, we have

$$(a^\dagger a)a |n\rangle = a(a^\dagger a - 1) |n\rangle = (n - 1)a |n\rangle, \quad (3.23)$$

$$(a^\dagger a)a^\dagger |n\rangle = a^\dagger(a^\dagger a + 1) |n\rangle = (n + 1)a^\dagger |n\rangle. \quad (3.24)$$

In other words, $a |n\rangle$ and $a^\dagger |n\rangle$ are eigenstates of N with eigenvalues $(n - 1)$ and $(n + 1)$, respectively. It means that when a and a^\dagger operate on $|n\rangle$, they decrease and increase n by one unit, respectively, what is equivalent to say that there was a *destruction (annihilation)* or a *creation* of a quantum of energy $\hbar\omega$.

From Eq. (3.23), we have that $a |n\rangle$ and $|n - 1\rangle$ represent the same eigenvector with different eigenvalue. Thus, to normalize the states $|n\rangle$ for all values of n , we can write

$$\gamma a |n\rangle = |n - 1\rangle, \quad (3.25)$$

where γ is a normalization constant. Then, in order to compute it we simply write

$$|\gamma|^2 \langle n | a^\dagger a |n\rangle = \langle n - 1 | n - 1 \rangle = 1, \quad (3.26)$$

and, on the other hand, Eq. (3.16) gives

$$\langle n | a^\dagger a |n\rangle = n \langle n | n \rangle = n. \quad (3.27)$$

When combined, these two last equations imply that

$$|\gamma|^2 = \frac{1}{n}. \quad (3.28)$$

This implies that n cannot be negative, $n \geq 0$, since the norm is a positive quantity. Equation (3.25) then becomes

$$\frac{a}{\sqrt{n}} |n\rangle = |n - 1\rangle, \quad (3.29)$$

and we can conclude that

$$a |n\rangle = \sqrt{n} |n-1\rangle. \quad (3.30)$$

A similar procedure is followed in order to find the action of a^\dagger on $|n\rangle$, which generates $|n+1\rangle$ (i.e., a^\dagger raises the eigenvalue by one unity). It can be easily shown that

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle. \quad (3.31)$$

The operators described in Eqs. (3.30) and (3.31) are also known as *lowering* and *raising* operators, respectively. When $n = 0$, we call $|0\rangle$ the **vacuum** state, or fundamental state, and it is defined by

$$a |0\rangle = 0. \quad (3.32)$$

All states after that can be build by applying a^\dagger on the vacuum state successively:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle. \quad (3.33)$$

It is easy to prove that the states $|n\rangle$ form an orthonormal basis, $\langle n|m\rangle = \delta_{n,m}$. They are also called **Fock states**, in honor of soviet physicist Vladimir Fock [108].

3.2.2 Coherent States Representation

The *coherent state* concept was first introduced by E. Schrödinger in 1926 [109]. Later, in the 1960s, John R. Klauder expressed these states as eigenvectors of the lowering operator [110]. After this, in 1963, Roy J. Glauber offered an excellent treatment of this subject in the quantum theory of light [111].

Conceptually speaking, a coherent state is a very specific quantum state, described in the context of the harmonic quantum oscillator, which refers to the state of a quantized electromagnetic field that most closely approximates a classical harmonic oscillator. It is a state characterized by a displacement of the ground-state wavepacket, that maximizes the coherence, i.e, it is a **minimum uncertainty state** [112].

Definition 4. We define a minimum uncertainty state $|\alpha\rangle$, which satisfies

$$a |\alpha\rangle = \alpha |\alpha\rangle \quad , \quad \alpha \in \mathbb{C} , \quad (3.34)$$

also known as a **coherent state** [113].

Here, the coherent state $|\alpha\rangle$ is the eigenvector of the annihilation operator. Since this operator is not Hermitian, the coherent states are not orthogonal, neither are

the eigenvalues real. In the following topics, we are going to describe some important properties of the coherent states which will be often needed.

i) Coherent states in terms of Fock states

In the Fock state basis, also called the number state $|n\rangle$, the coherent states takes the form

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \quad (3.35)$$

where $|\alpha|^2 = \alpha\alpha^*$. Then, the coherent states can be rewritten as

$$|\alpha\rangle = e^{\alpha a^\dagger - |\alpha|^2/2} |0\rangle. \quad (3.36)$$

ii) Displacement of the vacuum state

This can also be written in terms of a *displacement operator* $D(\alpha) = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{\alpha^* a}$, that operates on the vacuum state as

$$|\alpha\rangle = D(\alpha) |0\rangle, \quad (3.37)$$

since $e^{-\alpha^* a} |0\rangle = |0\rangle$. Using the Baker–Campbell–Hausdorff formula² for any two operators A and B , it may be shown that, if $[[A, B], A] = [[A, B], B] = 0$, then [114]

$$e^{A+B} = e^{-[A,B]/2} e^A e^B. \quad (3.38)$$

Therefore, it follows that

$$D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}. \quad (3.39)$$

The reason why the displacement operator is called this way is not very obvious at first glance. To understand this name, let us consider some of its properties. First, we can verify from Eq. (3.39) that

$$D^\dagger(\alpha)D(\alpha) = D(\alpha)D^\dagger(\alpha) = 1, \quad (3.40)$$

i.e, it is unitary, and also $D^\dagger(\alpha) = D(-\alpha)$, what means that if you displace the state by a given α and then do the opposite (displace back by $-\alpha$), you get the same result from the beginning. Secondly, the action of this operator on the annihilation operator results in

$$D^\dagger(\alpha)aD(\alpha) = e^{\alpha^* a - \alpha a^\dagger} a e^{\alpha a^\dagger - \alpha^* a}. \quad (3.41)$$

²See Appendix B.

If $a = B$ and $C = \alpha^* a - \alpha a^\dagger$, we can use the BCH formula

$$e^C B e^{-C} = B + [C, B] + \frac{1}{2!}[C, [C, B]] + \frac{1}{3!}[C, [C, [C, B]]] + \dots \quad (3.42)$$

and the commutation relation, $[a, a^\dagger] = 1$, in order to get

$$[\alpha^* a - \alpha a^\dagger, a] = \alpha. \quad (3.43)$$

Since as this is proportional to the identity, all higher order commutators in the BCH expansion will be zero. Therefore, we can write

$$D^\dagger(\alpha) a D(\alpha) = a + \alpha, \quad (3.44)$$

or, in other words, what the displacement operator does in fact is to displace the operator by an amount of α . That is the reason for its name. Likewise, since $D^\dagger(\alpha) = D(-\alpha)$ it follows that in the opposite displacement,

$$D(\alpha) a D^\dagger(\alpha) = a - \alpha. \quad (3.45)$$

In the case of the creation operator a^\dagger , we get that $D^\dagger(\alpha) a^\dagger D(\alpha) = a^\dagger + \alpha^*$.

iii) Orthogonality and completeness

To analyse the orthogonality of two coherent states α and β , let us compute its scalar product using the expression in Eq. (3.36):

$$\langle \beta | \alpha \rangle = e^{-|\beta|^2/2} e^{-|\alpha|^2/2} \langle 0 | e^{\beta^* a} e^{\alpha a^\dagger} | 0 \rangle. \quad (3.46)$$

Using now Eq. (3.38), we obtain

$$e^{\beta^* a} e^{\alpha a^\dagger} = e^{\alpha a^\dagger} e^{\beta^* a} e^{\beta^* \alpha}. \quad (3.47)$$

Thus, the scalar product can be written as

$$\langle \beta | \alpha \rangle = \exp \left(\beta^* \alpha - \frac{|\beta|^2}{2} - \frac{|\alpha|^2}{2} \right), \quad (3.48)$$

and the overlap between both states is given by

$$|\langle \beta | \alpha \rangle|^2 = \exp(-|\alpha - \beta|^2). \quad (3.49)$$

In other words, two coherent states are **not** orthogonal to each other, since the overlap between them decays exponentially. However, if α and β have a large difference from each other, they can be considered almost orthogonal. In the limit where $\alpha = \beta$,

$$\langle \alpha | \alpha \rangle = 1. \quad (3.50)$$

The coherent states obeys the completeness relation

$$\mathbf{1} = \frac{1}{\pi} \int d^2\alpha |\alpha\rangle \langle \alpha|, \quad (3.51)$$

where the integral is over the complex plane, $\alpha = \alpha_x + i\alpha_y$ and $d^2\alpha = d\alpha_x d\alpha_y$. Since there is a factor $1/\pi$ in front of the integral, and the coherent states are not orthogonal for different α and β , we say that the set of coherent states are *over-complete*.

iv) Coordinate and momentum spaces

Let's consider a class of quantum-mechanical systems described in the canonical coherent states basis, $|\alpha\rangle$, defined as the *eigenstates* of the annihilation operator of the harmonic oscillator described in Eq. (3.34) [115]. From Eqs. (3.13), one can rewrite this operator as

$$a = \frac{1}{2} \frac{q}{\sigma_q} + \frac{i}{2} \frac{p}{\sigma_p}, \quad (3.52)$$

where the uncertainties σ_q and σ_p of the respective operators q and p , computed in the ground state $|0\rangle$ of the harmonic oscillator, are given by

$$\sigma_q = \sqrt{\hbar/2m\omega} \quad \text{and} \quad \sigma_p = \sqrt{\hbar m\omega/2}. \quad (3.53)$$

Here, m is the mass of the particle and ω is the oscillator's angular frequency. The product between the uncertainties obeys the Heisenberg uncertainty relation [18],

$$\sigma_q \sigma_p = \frac{\hbar}{2}. \quad (3.54)$$

Thus, we have that the coordinate and momentum operators may be rewritten in terms of the annihilation and creation operators as

$$q = \sigma_q(a^\dagger + a), \quad \text{and} \quad p = i\sigma_p(a^\dagger - a). \quad (3.55)$$

The eigenvalues α and α^* can also be written as

$$\alpha = \frac{1}{2} \left(\frac{q}{\sigma_q} + \frac{ip}{\sigma_p} \right), \quad \text{and} \quad \alpha^* = \frac{1}{2} \left(\frac{q}{\sigma_q} - \frac{ip}{\sigma_p} \right). \quad (3.56)$$

The set of states $\{|\alpha\rangle\}_{\alpha \in \mathbb{C}}$ constitute an over-complete basis and obey the completeness rule

$$\mathbf{1} = \int d^2\alpha |\alpha\rangle \langle\alpha|,$$

where $d^2\alpha = d\alpha^* d\alpha / 2\pi i = dqdp / 2\pi\hbar$ is the volume element in the phase space and the projector onto a coherent state is $|\alpha\rangle \langle\alpha|$.

A coordinate transformation may be defined and it will be often needed. Here, we will identify the phase space plane of classical systems characterized by the canonical pair (q, p) as Ξ_{qp} , and the complex plane described by the conjugate pair (α, α^*) of the eigenvalues as Ξ_α . From Eq. (3.55), we can set expressions for q and p in terms of the eigenvalues as

$$q \equiv \langle\alpha|q|\alpha\rangle = \sigma_q(\alpha^* + \alpha) = 2\sigma_q \text{Re}(\alpha), \quad (3.57)$$

$$p \equiv \langle\alpha|p|\alpha\rangle = i\sigma_p(\alpha^* - \alpha) = 2\sigma_p \text{Im}(\alpha). \quad (3.58)$$

Here, $\text{Re}(\alpha)$ and $\text{Im}(\alpha)$ are the real and imaginary parts of α , respectively. Partial derivatives with respect to the coordinates of each pair can be written as

$$\partial_q = \frac{1}{2\sigma_q}(\partial_\alpha + \partial_{\alpha^*}), \quad \partial_p = \frac{i}{2\sigma_p}(\partial_\alpha - \partial_{\alpha^*}), \quad (3.59)$$

$$\partial_\alpha = \sigma_q \partial_q - i\sigma_p \partial_p, \quad \partial_{\alpha^*} = \sigma_q \partial_q + i\sigma_p \partial_p. \quad (3.60)$$

where we used a short-hand notation for the partial derivatives for the sake of simplicity.

v) The density operator

Consider the fluctuating classical field as a function of time for a field with large fluctuations, described in terms of a probability distribution $P(E)$ for the complex field amplitude $E = |E|e^{i\phi}$. In the statistical approach, we suppose that the system is in the state $|\psi\rangle$, and then the field is described by the density operator

$$\rho = \sum_{\psi} P_{\psi} |\psi\rangle \langle\psi|, \quad (3.61)$$

where P_ψ is the probability of being in the state $|\psi\rangle$. Then, any field operator O has the expectation value given by

$$\langle O \rangle = \text{Tr}(O\rho). \quad (3.62)$$

In terms of the photon occupation number states [107], we have

$$\rho = \sum_{n,m} |n\rangle \langle n| \rho |m\rangle \langle m| = \sum_{n,m} \rho_{nm} |n\rangle \langle m|, \quad (3.63)$$

or, by expanding in terms of coherent states,

$$\rho = \int \int \frac{d^2\alpha}{\pi} \frac{d^2\beta}{\pi} |\alpha\rangle \langle \alpha| \rho |\beta\rangle \langle \beta|. \quad (3.64)$$

3.2.3 The Husimi representation

Although the Wigner function was one of the first representations of the quantum phase space, other quasiprobability distributions have been highlighted over the years, in different contexts. Its most varied applications, ranging from quantum decoherence [116, 117], the interface between classical and quantum mechanics [118, 119], and even in chemistry [120, 121, 122], enabled the construction of a very useful mathematical apparatus in different areas of knowledge. One of these representations was Husimi's function, also known as *Q-function*, developed in the 1940s [123] and often used in quantum optics [124], more specifically in quantum tomography [125], and in the study of superconductor quantum effects [126]. Furthermore, Husimi's distribution has the advantage of being a positive function by definition.

The Husimi Q-distribution

Definition 5. *The Husimi function in the coherent state representation is defined as a quasi-distribution function corresponding to a density operator ρ as [107, 127]*

$$Q(\alpha, \alpha^*) = \frac{1}{\pi} \langle \alpha | \rho | \alpha \rangle, \quad (3.65)$$

where ρ is the density matrix of the system. From this definition, we see that the *Q-function* is positive definite. The normalization of $Q(\alpha, \alpha^*)$ is given by the normalization of the density operator,

$$1 = \text{Tr}\{\rho\} = \text{Tr}\left\{\frac{1}{\pi} \int d^2\alpha |\alpha\rangle \langle \alpha| \rho\right\} = \frac{1}{\pi} \int d^2\alpha \langle \alpha | \rho | \alpha \rangle, \quad (3.66)$$

such that

$$\int d^2\alpha Q(\alpha, \alpha^*) = 1. \quad (3.67)$$

In the case of a pure one-particle quantum state $|\varphi\rangle$ with projection $\varphi(\alpha, \alpha^*) = \langle\alpha|\varphi\rangle$, the associated Husimi function will be

$$Q_\varphi(\alpha, \alpha^*) = \frac{1}{\pi} |\varphi(\alpha, \alpha^*)|^2 = \text{Tr}(\rho |\alpha\rangle \langle\alpha|). \quad (3.68)$$

Expectation values of operators

Knowing the Q-function, one can also compute expectation values of operators. Let us obtain, for instance, the average of the creation operator that acts on the coherent state such that

$$\langle\alpha| a^\dagger = \langle\alpha| \alpha^*. \quad (3.69)$$

Thus, it follows that

$$\langle a^\dagger \rangle = \text{Tr}(a^\dagger \rho) = \frac{1}{\pi} \int d^2\alpha \langle\alpha| a^\dagger \rho |\alpha\rangle = \int d^2\alpha Q(\alpha, \alpha^*) \alpha^* \quad (3.70)$$

In fact, the expectation value of any operator T can be written as

$$\langle T \rangle = \text{Tr}(\rho T) = \frac{1}{\pi} \int d^2\alpha \langle\alpha| \rho T |\alpha\rangle = \int d^2\alpha Q(\alpha, \alpha^*) \mathcal{T}(\alpha, \alpha^*). \quad (3.71)$$

Examples of Husimi's functions

Next, we will describe how the calculation of Husimi functions is done given different quantum states and their respective density operators.

i) Coherent state

For a coherent state denoted by $|\beta\rangle$, the density operator is $\rho = |\beta\rangle \langle\beta|$ and we get

$$Q(\alpha, \alpha^*) = \frac{1}{\pi} \langle\alpha|\beta\rangle \langle\beta|\alpha\rangle = \frac{1}{\pi} |\langle\alpha|\beta\rangle|^2 = \frac{1}{\pi} \exp(-|\alpha - \beta|^2), \quad (3.72)$$

where we used the result obtained in Eq. (3.49). This is a Gaussian function in the complex plane, centered around β . When $\beta = 0$, we have the vacuum state, or ground-state of the harmonic oscillator (Fig. 3.3), by considering $\alpha = x + iy$ and $x = \text{Re}(\alpha)$, $y = \text{Im}(\alpha)$. The exponential form of this expression shows that $Q(\alpha, \alpha^*)$ will be significantly small, almost zero, unless $\beta \approx \alpha$, where the Q-function approximates $1/\pi$.

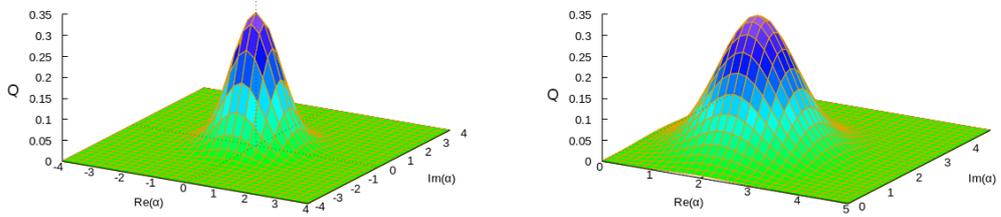


FIGURE 3.3: Q-function for the coherent state when $\beta = 0$ (left) and $\beta = 2 + 2i$ (right) in the 3D representation.

ii) Fock state

In this case, the state is represented by the number state defined in Eq. (3.33), then the density operator is given by $\rho = |n\rangle \langle n|$ and

$$Q_n(\alpha, \alpha^*) = \frac{1}{\pi} |\langle \alpha | n \rangle|^2 = \frac{1}{\pi} \exp(-|\alpha|^2) \frac{(|\alpha|^2)^n}{n!}. \quad (3.73)$$

Here, the Q-function has a maximum at $|\alpha|^2 = n$. The plots of Eq. (3.73) for $n = 1$ and $n = 5$ are given in Fig. 3.4.

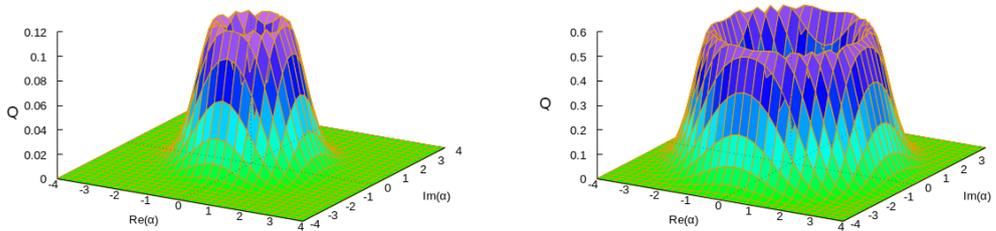


FIGURE 3.4: Q-function for the Fock state when $n = 1$ and $n = 5$, in the 3D representation.

iii) Thermal state

Let us now consider a thermal state (also called Gibbs state) given by

$$\rho_T = \frac{\exp(-\hbar\omega a^\dagger a / k_B T)}{Z}. \quad (3.74)$$

$Z = [1 - \exp(-\hbar\omega / k_B T)]^{-1}$ is the partition function, k_B is the Boltzmann constant and T is the temperature. Thus, we can write

$$\rho_T = (1 - e^{-\hbar\omega / k_B T}) e^{-\frac{\hbar\omega}{k_B T} a^\dagger a} = (1 - e^{-\hbar\omega / k_B T}) e^{-\frac{\hbar\omega}{k_B T} N}, \quad (3.75)$$

or, by introducing the identity operator $\hat{1} = \sum_n |n\rangle \langle n|$, we can also write

$$\rho_T = (1 - e^{-\hbar\omega/k_B T}) \sum_{n=0}^{\infty} |n\rangle \langle n| e^{-\frac{n\hbar\omega}{k_B T}}. \quad (3.76)$$

Substituting this last expression in the Q-function definition, we get

$$Q_T(\alpha, \alpha^*) = \frac{(1 - e^{-\hbar\omega/k_B T})}{\pi} \sum_{n=0}^{\infty} e^{-\frac{n\hbar\omega}{k_B T}} \langle \alpha | n \rangle \langle n | \alpha \rangle. \quad (3.77)$$

Now, from Eq. (3.73), we can rewrite this last expression as

$$Q_T(\alpha, \alpha^*) = \frac{(1 - e^{-\hbar\omega/k_B T})}{\pi} \sum_{n=0}^{\infty} e^{-\frac{n\hbar\omega}{k_B T}} \exp(-|\alpha|^2) \frac{(|\alpha|^2)^n}{n!}, \quad (3.78)$$

so that

$$Q_T(\alpha, \alpha^*) = \frac{(1 - e^{-\hbar\omega/k_B T})}{\pi} \exp[-|\alpha|^2 (1 - e^{-\hbar\omega/k_B T})]. \quad (3.79)$$

At large temperatures, we can approximate the exponential factor to get

$$Q_T(\alpha, \alpha^*) \rightarrow \frac{\hbar\omega}{\pi k_B T} \exp\left(-\frac{\hbar\omega|\alpha|^2}{k_B T}\right). \quad (3.80)$$

This last expression reminds a lot of a Boltzmann distribution.

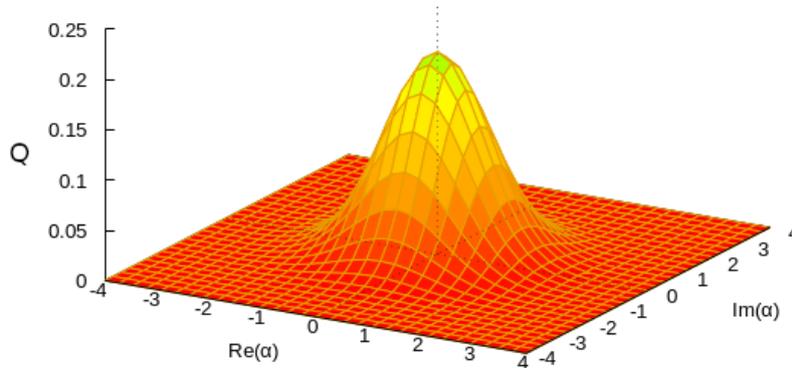


FIGURE 3.5: Q-function for the thermal state when we set $\hbar = \omega = k_B = T = 1$ in the 3D representation.

iv) Schrödinger cat state

If we have a superposition of states such as

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\phi\rangle + |-\phi\rangle), \quad (3.81)$$

we called it a Schrödinger cat state, where ϕ represents a coherent state. From the result of the scalar product obtained in Eq. (3.48), we then get

$$Q_{cat}(\alpha, \alpha^*) = \frac{1}{\pi} e^{-|\alpha-\phi|^2} \left(1 + \frac{e^{-2\phi^*\alpha} + e^{-2\phi\alpha^*}}{2} \right). \quad (3.82)$$

v) Squeezed states

When a quantum state has minimal uncertainty concerning a physical variable, for example, if the product of the dispersions of q and p reaches the minimum value established by the Heisenberg uncertainty relation, $\hbar/2$, we have what it is called a coherent state. The squeezed state is a generalization of the coherent states and it very useful in many applications in quantum optics, especially due to the possibility of increasing the precision in measurements. The idea is to decrease (squeeze) the uncertainty in one quadrature with the cost of increasing it in the other.

A squeezed coherent state is defined by the application of a displacement operator $D(\beta)$ similar of that in Eq. (3.39), on the vacuum state $|0\rangle$ followed by the unitary squeeze operator [107],

$$S(\zeta) = \exp\left(\frac{1}{2}\zeta^* a^2 - \frac{1}{2}\zeta a^{\dagger 2}\right), \quad (3.83)$$

where $\zeta = r e^{i\theta}$ is a complex number chosen arbitrarily and r is a squeezing parameter. Therefore, we get

$$|\beta, \zeta\rangle = S(\zeta) D(\beta) |0\rangle. \quad (3.84)$$

Here, $\beta = |\beta| e^{i\varphi}$ and $S^\dagger(\zeta) = S^{-1}(\zeta) = S(-\zeta)$. From BCH formula in Eq. (3.42), we get the following transformations for the annihilation and creation operators

$$S^\dagger(\zeta) a S(\zeta) = a \cosh r - a^\dagger e^{i\theta} \sinh r, \quad (3.85)$$

$$S^\dagger(\zeta) a^\dagger S(\zeta) = a^\dagger \cosh r - a e^{-i\theta} \sinh r. \quad (3.86)$$

The associated density operator is given by

$$\rho_S = S(\zeta) |\beta\rangle \langle\beta| S^\dagger(\zeta), \quad (3.87)$$

where we used the definition in Eq. (3.37), and $|\beta\rangle = D|0\rangle$. Hence, the Q -function will be

$$Q_S(\alpha, \alpha^*) = \frac{1}{\pi} \langle\alpha|\beta, \zeta\rangle \langle\beta, \zeta|\alpha\rangle = \frac{1}{\pi} |\langle\alpha|\beta, \zeta\rangle|^2. \quad (3.88)$$

Therefore, all we need to do is find the function $\langle\alpha|\beta, \zeta\rangle$ using the properties of the coherent states and the relations in Eqs. (3.85) and (3.86). This calculation is described in detail in Section 3.5 of the excellent book *Quantum Optics*, by Scully and Zubairy [107], and for the sake of simplicity, we will only present the final result. Then, we have that the Q -representation for the state $|\beta, \zeta\rangle$ is given by

$$Q_S(\alpha, \alpha^*) = \frac{\text{sech}r}{\pi} \exp\{-(|\alpha|^2 + |\beta|^2) + (\alpha^*\beta + \beta^*\alpha)\text{sech}r - \frac{1}{2}[e^{i\theta}(\alpha^{*2} - \beta^{*2}) + e^{-i\theta}(\alpha^2 - \beta^2)]\text{tanh}r\}. \quad (3.89)$$

The Husimi flow

In the section on classical mechanics, we saw that the evolution of the system and particle trajectories in phase space could be analysed using Hamilton's equations, and thus the entire dynamics of the system would be represented by a continuity equation. In that case, we had a generalized function $F(q, p; t)$ and a phase space current described by \mathbf{J} . The continuity equation was Liouville's equation. By precisely defining the phase space currents for each variable, we obtained the flow of $F(q, p; t)$ and all the dynamics necessary to understand how the system evolves in time.

At this stage of the work, we will use the Husimi Q -function as a starting point to describe the flow of the quantum phase space through a very similar continuity equation, the Liouville-Von Neumann equation. The latter arises naturally when obtaining the equations of motion for a density matrix and the time-dependent Schrodinger equation.

If the Q -function depends on time we write

$$Q_\varphi(\alpha, \alpha^*, t) = \text{Tr}(|\alpha\rangle \langle\alpha| \rho(t)), \quad (3.90)$$

where the time evolution is governed by

$$\rho(t) = U(t)\rho_0U^\dagger(t), \quad (3.91)$$

and $\rho_0 = \rho(0)$. The time evolution operator when the Hamiltonian does not depend on time is simply [72]

$$U(t, t_0) = e^{Ht/i\hbar}. \quad (3.92)$$

Therefore, the dynamics of the Husimi function will be given by the following differential equation

$$i\hbar \frac{\partial}{\partial t} Q_\varphi = \text{Tr}(|\alpha\rangle\langle\alpha|H\rho) - \text{Tr}(\rho H^\dagger|\alpha\rangle\langle\alpha|), \quad (3.93)$$

where we used the Liouville-von Neumann relation [74],

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}[H, \rho] = \frac{1}{i\hbar}(H\rho - \rho H^\dagger), \quad (3.94)$$

and the linearity of the trace. Thus, we should get the trace of the product between the projector $|\alpha\rangle\langle\alpha|$ and the relation between ρ and H . This is obtained through a differential algebra on the representation of coherent states [128, 113], and it was performed in greater detail in the references [17, 129], where it was assumed that the Hamiltonian could be represented by a normal ordered power series of the annihilation and creation operators,

$$H = \sum_{m,n} c_{mn} a^{\dagger m} a^n, \quad (3.95)$$

and if $c_{mn} = c_{nm}^*$ the Hamiltonian is Hermitian. In the coherent states representation the normalized matrix elements of H would be written as

$$H(\alpha'^*, \alpha) = \frac{\langle\alpha'|H|\alpha\rangle}{\langle\alpha'|\alpha\rangle} = \sum_{m,n} c_{mn} \alpha'^{*m} \alpha. \quad (3.96)$$

From the formulation of Q -function representation given in the book *Quantum noise*, by Gardiner and Zoller [127], we get that the following set of relations hold

$$\begin{aligned} a\rho &\leftrightarrow \left(\alpha + \frac{\partial}{\partial\alpha^*}\right) Q(\alpha, \alpha^*), & a^\dagger\rho &\leftrightarrow \alpha^* Q(\alpha, \alpha^*), \\ \rho a^\dagger &\leftrightarrow \left(\alpha^* + \frac{\partial}{\partial\alpha}\right) Q(\alpha, \alpha^*), & \rho a &\leftrightarrow \alpha Q(\alpha, \alpha^*). \end{aligned} \quad (3.97)$$

Applying Eq. (3.97) to the dynamics described in Eq. (3.93), with the general Hamiltonian in Eq (3.95), we have

$$\text{Tr}(|\alpha\rangle \langle \alpha| H \rho) = \sum_{m,n} c_{mn} \alpha^{*m} \left(\alpha + \frac{\partial}{\partial \alpha^*} \right)^n Q_\varphi. \quad (3.98)$$

For the second term in the differential equation (3.93) we use the same procedure, and after substituting these results we obtain the following equation

$$i\hbar \frac{\partial}{\partial t} Q_\varphi = \sum_{m,n} \left[c_{mn} \alpha^{*m} \left(\alpha + \frac{\partial}{\partial \alpha^*} \right)^n - c_{mn}^* \alpha^m \left(\alpha^* + \frac{\partial}{\partial \alpha} \right)^n \right] Q_\varphi. \quad (3.99)$$

In order to write the continuity equation in phase space for the Q -function, we have to recast Eq. (3.99) in such a way that we find an equivalent current \mathbf{J} in a similar way we did in the classical case. Thus, from Eq. (3.6) we know that the continuity equation can be restated in terms of the Poisson bracket between H and F as

$$\frac{\partial F}{\partial t} = \{H, F\}_{\mathbb{R}} \quad \text{for } \Xi_{qp}, \quad (3.100)$$

or, by changing coordinates and using the transformations in Eqs. (3.58) and (3.58), we can rewrite this expression in the complex plane Ξ_α as

$$\{H, F\}_{\mathbb{R}} = \frac{1}{i\hbar} \{H, F\}_{\mathbb{C}} \quad \text{for } \Xi_\alpha, \quad (3.101)$$

where

$$\{H, F\}_{\mathbb{C}} = \left(\frac{\partial H}{\partial \alpha} \frac{\partial F}{\partial \alpha^*} - \frac{\partial H}{\partial \alpha^*} \frac{\partial F}{\partial \alpha} \right). \quad (3.102)$$

Therefore, the Hamilton's equation of motion will be

$$i\hbar \begin{pmatrix} \frac{d\alpha}{dt} \\ \frac{d\alpha^*}{dt} \end{pmatrix} = \mathbf{M}_2 \begin{pmatrix} \frac{\partial H}{\partial \alpha} \\ \frac{\partial H}{\partial \alpha^*} \end{pmatrix}, \quad (3.103)$$

and then, the classical currents in the Ξ_α , when $F = Q(\alpha, \alpha^*)$, are given by

$$J_{cl,\alpha} = Q \frac{d\alpha}{dt} = \frac{Q}{i\hbar} \frac{\partial H}{\partial \alpha^*} \quad \text{and} \quad J_{cl,\alpha^*} = Q \frac{d\alpha^*}{dt} = -\frac{Q}{i\hbar} \frac{\partial H}{\partial \alpha}. \quad (3.104)$$

These last expressions are, of course, classical limits. They naturally arise from a broader formulation of the analytical expression for the Husimi's current given by

$$J_\alpha = \frac{1}{i\hbar} \sum_{l=1} \frac{\partial^{l-1} Q}{\partial \alpha^{l-1}} \sum_{k=0} \frac{(-1)^k}{(k+l)!} \frac{\partial^{2k+l} H^*}{\partial \alpha^{*(k+l)} \partial \alpha^k}, \quad (3.105)$$

and a similar expression for $J_{\alpha^*} = J_{\alpha}^*$. This calculation is presented in details in Ref. [17] by considering a quantum continuity equation written as

$$\frac{\partial}{\partial t} Q_{\varphi} = -\nabla \mathbf{J} = -\frac{\partial}{\partial \alpha} J_{\alpha} - \frac{\partial}{\partial \alpha^*} J_{\alpha^*}. \quad (3.106)$$

Therefore, after applying expansions in the derivatives in Eq. (3.99) and other calculations that we are not going to explicit show here for the sake of simplicity, the authors of the mentioned reference established a correspondence between the two equations for the flow, and the consequent definition of the currents J_{α} and J_{α^*} in quantum phase space. In the correspondent Ξ_{qp} space, we get that

$$J_q = \sigma_q (J_{\alpha^*} + J_{\alpha}) = 2\sigma_q \operatorname{Re}(J) \quad (3.107)$$

$$J_p = i\sigma_p (J_{\alpha^*} - J_{\alpha}) = 2\sigma_p \operatorname{Im}(J). \quad (3.108)$$

Chapter 4

Thermodynamic uncertainty relation for the Husimi Q-function

So far, we have made a theoretical review of thermodynamic uncertainty relations and their meaning, and we have explained the quantum context of the phase space, defining the Husimi flux in the representation of coherent states, as these are states that minimize uncertainty. Now, we are finally ready to design a TUR for the flow in phase space and understand what kind of information this gives us.

4.1 Derivation of the TUR in phase space

The main idea behind this approach, as seen before in Chapter 2, is to evoke the Cramér-Rao bound, which gives us a fundamental relation between the variance of the estimator of a fixed parameter, which in our case will be the Husimi current, and the Fisher information. Moreover, since we can have two currents, we look for the covariance measure between them, and the estimator considered here is defined as unbiased, because we want to achieve the lowest possible bound.

4.1.1 Cramér-Rao bound

The Cramér-Rao bound for an unbiased estimator J reads [130, 131]

$$\Delta_J \geq \frac{1}{\mathcal{F}}, \quad (4.1)$$

where Δ_J is the mean square root error, or the uncertainty of a general estimation process, and \mathcal{F} is the Fisher information, which is defined as

$$\mathcal{F}(\theta) = \int d\mathbf{x} f_\theta(\mathbf{x}) \left\{ \frac{\partial \ln f_\theta(\mathbf{x})}{\partial \theta} \right\}^2, \quad (4.2)$$

with $f_\theta(\mathbf{x})$ being a probability distribution function, and $\theta \in \mathbb{R}$ is some parameter to be estimated. In the case of distribution functions whose form does not change under θ displacements (shift invariant), we can write

$$\mathcal{F} = \int d\mathbf{x} f(\mathbf{x}) \left\{ \frac{\partial \ln f(\mathbf{x})}{\partial \mathbf{x}} \right\}^2. \quad (4.3)$$

Fisher information gives us a measurement of the amount of information about the required parameter that is encoded in the state of the system. Therefore, it quantifies the uncertainty in the estimation of the parameter. As we can see, \mathcal{F} depends on the probability distribution $f_\theta(\mathbf{x})$ and the derivative $\partial(\ln f_\theta(\mathbf{x}))/\partial\theta$, which is known as the *score function*, and describes how sensitive f_θ is to changes in θ given a particular value of θ . Moreover, what Eq. (4.2) tells us is the overall sensitivity of f_θ to changes of θ by calculating its weight at each outcome \mathbf{x} with respect to the chance given in $f_\theta(\mathbf{x})$. In the next section, we will see that the Fisher information is also described as the variance of the score function, what is essential to obtain the Cramér-Rao bound.

Proof of CRB for an unbiased estimator

By using the Cauchy–Schwarz inequality [132], we can show that there is a covariance inequality given by

$$\text{Cov}(A, B)^2 \leq \text{Var}(A)\text{Var}(B), \quad (4.4)$$

where A and B can be any random variables, and Cov and Var denote *covariance* and *variance*, respectively. In terms of the expected values,

$$\text{Cov}(A, B) = \langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle. \quad (4.5)$$

If A is the *score function* given by

$$A \equiv \frac{\partial}{\partial \theta} \ln f_\theta(\mathbf{x}) = \frac{\frac{\partial}{\partial \theta} f_\theta(\mathbf{x})}{f_\theta(\mathbf{x})}, \quad (4.6)$$

the variance of the score, $\text{Var}(A) = \langle A^2 \rangle$ is the measure we call *Fisher information* $\mathcal{F}(\theta)$,

$$\mathcal{F}(\theta) \equiv \left\langle \frac{\partial}{\partial \theta} \ln f_\theta(\mathbf{x}) \right\rangle^2. \quad (4.7)$$

Also, the mean value of the score is zero,

$$\langle A \rangle = \int A f_\theta(\mathbf{x}) d\mathbf{x} = \int \frac{\frac{\partial}{\partial \theta} f_\theta(\mathbf{x})}{f_\theta(\mathbf{x})} f_\theta(\mathbf{x}) d\mathbf{x} \quad (4.8)$$

$$= \frac{\partial}{\partial \theta} \int f_\theta(\mathbf{x}) d\mathbf{x} = \frac{\partial}{\partial \theta} (1) = 0. \quad (4.9)$$

Let us assume that $B \equiv B(\theta)$ is an unbiased estimator, or in other words, that there's no difference between the true value of the parameter θ and the expected value, $\langle T \rangle = \theta$ for all θ . Therefore, the Cauchy-Schwarz inequality in Eq. (4.5), after some calculations, takes the form

$$\langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle^2 \leq \langle (A - \langle A \rangle)^2 \rangle \langle (B - \langle B \rangle)^2 \rangle \quad (4.10)$$

$$\langle AB \rangle^2 \leq \langle A^2 \rangle \langle B^2 \rangle. \quad (4.11)$$

Or, if $\langle A^2 \rangle = \text{Var}(A) = \mathcal{F}(\theta)$ and $\langle B^2 \rangle = \text{Var}(B)$,

$$\langle AB \rangle^2 \leq \mathcal{F}(\theta) \text{Var}(B). \quad (4.12)$$

Now we need to obtain the left side of this inequality. One can calculate it directly by using Eq. (4.6)

$$\langle AB \rangle = \int A B(\mathbf{x}) f_\theta(\mathbf{x}) d\mathbf{x} \quad (4.13)$$

$$= \frac{\partial}{\partial \theta} \int f_\theta(\mathbf{x}) B(\mathbf{x}) d\mathbf{x} = \frac{\partial}{\partial \theta} \langle B \rangle = \frac{\partial}{\partial \theta} \theta = 1 \quad (4.14)$$

$$\therefore \langle AB \rangle^2 = 1. \quad (4.15)$$

Substituting this results back into Eq. (4.12), we finally get

$$\mathcal{F}(\theta) \text{Var}(B) \geq 1, \quad (4.16)$$

which is the Cramér-Rao bound for any unbiased estimators we stated in Eq. (4.1).

4.1.2 Fisher information and the relative entropy

For our purposes, we will be interested in express the Fisher information of a quasiprobability Q_θ in terms of the calculation of the relative entropy between Q_θ and $Q_{\theta+\delta_\theta}$, which means that we are changing the parameter θ by a small amount δ_θ . In other words, the quantity δ_θ is a measure of the accuracy (minimum error) of the process under consideration. It gives us the information about how well can we tell apart

one quasiprobability distribution from another. In general, the relative entropy between these two distributions can be written as [133]

$$D(Q_\theta || Q_{\theta+\delta_\theta}) = \int Q_\theta \ln \frac{Q_\theta}{Q_{\theta+\delta_\theta}} d\theta. \quad (4.17)$$

After applying a Taylor expansion about δ_θ up to the second order, we can show that

$$D(Q_\theta || Q_{\theta+\delta_\theta}) \approx \frac{\delta_\theta^2}{2} \int Q_\theta \left(\frac{\partial}{\partial \theta} \ln Q_\theta \right)^2 d\theta = \frac{\delta_\theta^2}{2} \mathcal{F}(Q_\theta). \quad (4.18)$$

Therefore, we are allowed to express the Fisher information in terms of the relative entropy as

$$\mathcal{F} \approx \frac{2}{\delta_\theta^2} D(Q_\theta || Q_{\theta+\delta_\theta}). \quad (4.19)$$

Proof of Eq. (4.18)

From (4.17), we can apply a Taylor expansion about δ_θ

$$\ln Q_{\theta+\delta_\theta} - \ln Q_\theta = \delta_\theta \frac{\partial \ln Q_\theta}{\partial \theta} + \frac{\delta_\theta^2}{2} \frac{\partial^2 \ln Q_\theta}{\partial \theta^2} + \mathcal{O}(\delta_\theta^3). \quad (4.20)$$

Then, we can rewrite Eq. (4.17) as

$$D(Q_\theta || Q_{\theta+\delta_\theta}) = - \int Q_\theta (\ln Q_{\theta+\delta_\theta} - \ln Q_\theta) d\theta \quad (4.21)$$

$$\approx - \int \left(\delta_\theta \frac{Q_\theta}{Q_\theta} \frac{\partial Q_\theta}{\partial \theta} + \frac{\delta_\theta^2}{2} \frac{Q_\theta}{Q_\theta} \frac{\partial^2 \ln Q_\theta}{\partial \theta^2} \right) d\theta. \quad (4.22)$$

The first order term will be zero, since

$$- \delta_\theta \int \frac{\partial Q_\theta}{\partial \theta} d\theta = - \delta_\theta \frac{\partial}{\partial \theta} \int Q_\theta d\theta = 0. \quad (4.23)$$

The second order term is

$$- \frac{\delta_\theta^2}{2} \int \frac{\partial^2 \ln Q_\theta}{\partial \theta^2} d\theta = - \frac{\delta_\theta^2}{2} \int \frac{Q_\theta}{Q_\theta} \frac{\partial^2 Q_\theta}{\partial \theta^2} d\theta + \frac{\delta_\theta^2}{2} \int Q_\theta \left(\frac{1}{Q_\theta} \frac{\partial Q_\theta}{\partial \theta} \right)^2 d\theta. \quad (4.24)$$

However, the quasiprobability Q-distribution is normalized, which leads us to

$$\int \frac{\partial^2 Q_\theta}{\partial \theta^2} d\theta = 0. \quad (4.25)$$

Then, up to the second order we can write

$$D(Q_\theta || Q_{\theta+\delta_\theta}) \approx \frac{\delta_\theta^2}{2} \int Q_\theta \left(\frac{\partial}{\partial \theta} \ln Q_\theta \right)^2 d\theta, \quad (4.26)$$

or, in terms of the definition of the Fisher information, $\mathcal{F}(Q_\theta)$, results

$$D(Q_\theta || Q_{\theta+\delta_\theta}) \approx \frac{\delta_\theta^2}{2} \mathcal{F}(Q_\theta). \quad (4.27)$$

4.1.3 Connection with thermodynamics

As seen in Chapter 2, the relation between the probabilities concerning the forward and backward processes is described by the Crooks relation and the Jarzynski equality is the result of its direct integration. For our case, since the Q-function is a quasiprobability density that represents the phase-space distribution of a quantum state, we will assume that $Q_\theta \rightarrow Q_{eq}(q, p; t)$ plays the role of a state in equilibrium and the small variation on the parameter θ we are considering is connected to a nonequilibrium state such as $Q_{\theta+\delta_\theta} \rightarrow Q(q, p; t)$. In this set, we can define σ as the change in the entropy caused by taking the system out of equilibrium. It could be the dissipated work in the estimation process, for instance, but for now we are going to discuss just the general form of this relation and how it connects with relative entropy and the Fisher information. If we take the average of the quantity σ , we obtain

$$\langle \sigma \rangle \equiv \int Q(q, p; t) \ln \left[\frac{Q(q, p; t)}{Q_{eq}(q, p; t)} \right] dq dp, \quad (4.28)$$

or, in terms of the relative entropy, this can be rewritten as

$$\langle \sigma \rangle = D(Q(q, p; t) || Q_{eq}(q, p; t)). \quad (4.29)$$

Combining this result with Eq. (4.27), the Cramér-Rao bound can be written as

$$\frac{\Delta_J}{\delta^2} \langle \sigma \rangle \geq \frac{1}{2}, \quad (4.30)$$

and the uncertainty Δ_J can be written in terms of the Husimi current as

$$\Delta_J = \langle |J|^2 \rangle - \langle |J| \rangle^2. \quad (4.31)$$

Equation (4.30) can be interpreted as a thermodynamic uncertainty relation for currents in phase space using the Husimi representation, which is the main result of this dissertation. One can note that it is a bound similar to that obtained

in Refs. [16]. Furthermore, our result approximates that of reference [1] in the context of thermodynamic cost of acquiring information.

The TUR obtained tell us that we have a minimal cost in the value of the relative entropy, defined here in terms of the Husimi quasiprobability function, when we use for the estimator the phase-space current. In other words, this means that, in order to control current fluctuations near equilibrium by reducing their relative uncertainty Δ_J/δ^2 , there is a cost that must be paid as dissipated energy. Moreover, this is in agreement with the fluctuation-dissipation theorem [134].

4.2 Classical Husimi's Current

In terms of the covariance between two currents, where β is a coherent state, the covariance matrix is defined as

$$\text{Cov}_\beta(J_\alpha, J_{\alpha^*}) = \text{Tr}[J_\alpha J_{\alpha^*} \rho(\beta)] - \text{Tr}[J_\alpha \rho(\beta)] \text{Tr}[J_{\alpha^*} \rho(\beta)]. \quad (4.32)$$

This last one can be rewritten by setting

$$\text{Cov}_\beta(J_\alpha, J_{\alpha^*}) \equiv \Delta(J_\alpha, J_{\alpha^*}) = \langle J_\alpha J_{\alpha^*} \rangle - \langle J_\alpha \rangle \langle J_{\alpha^*} \rangle \quad (4.33)$$

$$\begin{aligned} &= \int d^2\alpha Q(\alpha, \alpha^*) J_\alpha J_{\alpha^*} + \\ &- \int d^2\alpha Q(\alpha, \alpha^*) J_\alpha \int d^2\alpha Q(\alpha, \alpha^*) J_{\alpha^*}. \end{aligned} \quad (4.34)$$

From Chapter 3, we remember that the Husimi current given in Eq. (3.105) can be written, in its lowest order current components, as

$$J_\alpha = \frac{Q}{i\hbar} \frac{\partial H^*}{\partial \alpha^*}, \quad J_{\alpha^*} = -\frac{Q}{i\hbar} \frac{\partial H}{\partial \alpha}. \quad (4.35)$$

These are general relations valid for any Hamiltonian.

4.2.1 Example: The Squeezed Oscillator

In Chapter 3, we introduced the concept of the *squeezed coherent state*, which is a generalization of the coherent states that describes a quantum state of minimal uncertainty. Now, in order to obtain the Hamiltonian and the Husimi current for these states, we need to consider coherent states with different uncertainties σ_q and σ_p on the respective operators q and p (see Eq. (3.53)). We already know that the coordinate and momentum operators can be written in terms of the annihilation and creation operators as in Eqs. (3.55). However, with different widths σ'_q and σ'_p ,

the annihilation operator may be rewritten as

$$a' = \frac{1}{2} \frac{q}{\sigma'_q} + \frac{i}{2} \frac{p}{\sigma'_p}. \quad (4.36)$$

Using the position and momentum operators defined in Eqs (3.55), we get

$$a' = \frac{1}{2} \left[\left(\frac{\sigma_q}{\sigma'_q} - \frac{\sigma_p}{\sigma'_p} \right) a^\dagger + \left(\frac{\sigma_q}{\sigma'_q} + \frac{\sigma_p}{\sigma'_p} \right) a \right]. \quad (4.37)$$

If we define the squeezing parameter r such that

$$\frac{\sigma_q}{\sigma'_q} = \frac{\sigma'_p}{\sigma_p} = e^r, \quad (4.38)$$

the new annihilation and creation operators will then be given by

$$a' = a^\dagger \sinh r + a \cosh r, \quad (4.39)$$

$$a'^\dagger = a^\dagger \cosh r + a \sinh r. \quad (4.40)$$

The Hamiltonian can be written as

$$H = \hbar\omega'(a'^\dagger a' + 1/2), \quad (4.41)$$

where the frequency is $\omega' = \sigma'_p/(m\sigma'_q) = e^{2r}\sigma_p/(m\sigma_q) = e^{2r}\omega$. Therefore, the Hamiltonian can be expressed as

$$H = \hbar\omega e^{2r} \left[\frac{1}{2}(a'^{\dagger 2} + a'^2) \sinh 2r + a'^\dagger a' \cosh 2r + \frac{1}{2} \cosh 2r \right]. \quad (4.42)$$

In the limit where $r \rightarrow 0$, the uncertainties σ'_q and σ'_p are the same as σ_q and σ_p . Also, Eq. (4.42) becomes

$$H = \hbar\omega(a^\dagger a + 1/2), \quad (4.43)$$

which is the Hamiltonian of the harmonic oscillator, as expected. The α -component of the Husimi current will then be given by

$$J_\alpha = -i\omega e^{2r} (\alpha^* \sinh 2r + \alpha \cosh 2r) Q - i\frac{\omega}{2} e^{2r} \sinh 2r \frac{\partial Q}{\partial \alpha}, \quad (4.44)$$

for the squeezed harmonic oscillator, and the currents associated to the Husimi flow in the semiclassical approximation of the harmonic oscillator will be given by

$$J_\alpha = -i\omega\alpha Q, \quad J_{\alpha^*} = i\omega\alpha^* Q. \quad (4.45)$$

In this last case, the Husimi function, Q , can assume different forms depending on the state we are dealing with. In the Appendix D, we have calculated $\Delta(J_\alpha, J_{\alpha^*})$ for the coherent state in Eq. (3.72), the Fock state in Eq. (3.73), and the thermal state in Eq. (3.79). However, these calculations led to a null result in the covariance between the two currents considered.

Chapter 5

Final Remarks

UNDERSTANDING the behavior of current fluctuations in the far from equilibrium thermodynamic processes allows us to better understand fundamental aspects of the laws of thermodynamics and their direct or indirect consequences in the development of new technological devices. The measurement of physical observables has a statistical nature, so the study of the probabilities involved is inherent to the entire process. Analyzing probability currents and their fluctuations leads us directly to ways to control the energy dissipation that is intrinsic to every interaction between systems and the environment. Realizing them from different points of view can be a powerful tool to complement a broader picture. In this work, we make a connection between different areas of physics that have conceptual definitions in different contexts, such as Statistical Physics (entropy), Information Theory (Fisher information) and Quantum Mechanics (quasiprobability distributions in the phase space formalism). Moreover, this is how new concepts and theories develop.

Starting from a thermodynamic view, we saw that the second law provides us with a fundamental threshold to the production of entropy, and how this defines what we call reversible and irreversible processes. For the latter, entropy production is always non-negative. However, in addition to not being negative, we also saw that it has a lower bound which is a non-zero constant. This, in turn, is directly related to the measurement accuracy of the observable in a given process. This is the seed that produces what we call the thermodynamic uncertainty relation, a relation between the averages of the entropy production of the current fluctuations and their respective relative uncertainties. We discussed examples in the classical and quantum worlds of how a TUR is obtained, according to research carried out recently.

After reviewing derivations of classical and quantum TURs, we showed how to define probability densities in the quantum phase space, thus providing another conceptual angle of irreversible processes, which lead us to the emergence of TUR also for probability current fluctuations characterized in the context of quantum information. For this, we chose the Husimi representation based on coherent states,

which has more intuitive interpretation properties and can be directly converted to classical coordinates of phase space. We obtained the quasiprobability function for different examples of states, intending to later apply them to the TUR under development.

There are different ways to obtain a TUR. The approach we chose was to use the Cramér-Rao bound, which sets a limit to the variance of an unbiased estimator of some fixed parameter in terms of the inverse of Fisher information. Such a technique has been previously applied to obtain a quantum TUR, as shown in Chapter 2. Fisher information is related to relative entropy, and consequently to the average of entropy production. The variance divided by the mean squared provides the other TUR term we need. With that in mind, in Chapter 4, the thermodynamic uncertainty relation for currents in phase space was finally obtained. In recent works, this current was calculated for a closed system, with temporal evolution described in terms of the von Neumann equation. In this system, the probability is conserved, so we can properly define a flux for it, the Husimi flux in phase space, as discussed in Chapter 3. The current changes according to the considered state, then we have applied the Husimi functions to coherent, Fock, Gibbs (thermal), coherent superposition (Schrodinger cat), and squeezed states, observing the shape of the curve that shows us that the Q-function is always positive, as expected. With these expressions for the different states, we have applied them in the definition of the classical Husimi current, obtaining the current variance, which gives us the relative uncertainty for the TUR in Eq. (4.30), and therefore, the lower bound in the average entropy production.

As an example, we have considered the classical current approximation, which resembles the current of a continuity equation. The current here was defined in terms of the Husimi function and the Hamiltonian function of the system, which in this case was the squeezed harmonic oscillator, which in a certain limit can be described also as the simple harmonic oscillator. Other systems and Hamiltonians could be used, however, we chose to analyze the simple harmonic oscillator first to see how our solution behaves. In a broader picture, we believe that the TUR can be extended to other systems, such as open quantum system which interact with some environment or systems under the action of stochastic perturbations.

Appendix A

Fluctuation Theorems

FLUCTUATION Theorem (FT) refer to a mathematical relation involving different probability densities of the entropy production of a given irreversible process over a certain time. Several FTs have been proposed in the last two decades, but in this work our attention has turned more specifically to two, described by the equations (2.1) and (2.2), which we will make a brief derivation below.

A.1 The Evans-Searles Fluctuation Theorem

At the following, we show a derivation for the FT described as

$$\frac{P(\Omega_t = A)}{P(\Omega_t = -A)} = \exp(A), \quad (\text{A.1})$$

where $P(\Omega_t)$ means the probability of observing trajectories in phase space, at a certain time t , with a entropy production Ω_t that assumes an arbitrary number A . This is valid for systems over a short time scale. There are several derivations of this FT, for instance by using deterministic dynamics [48] or even the stochastic approach [135]. Here, we will derive the FT using the first one, by following the logical order of theorem development. First, we discuss some concepts of phase space needed in this approach. Later, we obtain the FT by calculating the relative probability of the dissipation function concerning the different trajectories in phase space.

A.1.1 Hamiltonian dynamics and Liouville's Equation

Characterizing all the possible states of a Hamiltonian system in the phase space is a difficult task, since the number of particles of a typical system scales exponentially and it makes impossible to know their exact configurations. Therefore, in order to better describe these systems we use probability distribution functions. By denoting

$\Gamma = (q, p)$ as a point in phase space, and $f(\Gamma, t)$ as the probability distribution function, the probability of finding the system in an infinitesimal phase space volume $d\Gamma$ is

$$P(d\Gamma_t, t) \equiv f(\Gamma_t, t)d\Gamma_t. \quad (\text{A.2})$$

Calculating the total time derivative of f , we get

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial p}\dot{p} + \frac{\partial f}{\partial q}\dot{q} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \Gamma} \cdot \dot{\Gamma}. \quad (\text{A.3})$$

For the probability flow in the phase space, the continuity equation holds, then

$$\frac{\partial(f\dot{\Gamma})}{\partial \Gamma} + \frac{\partial f}{\partial t} = 0. \quad (\text{A.4})$$

We can eliminate the partial derivative of t , obtaining

$$\frac{df}{dt} = -f \frac{\partial \dot{\Gamma}}{\partial \Gamma}. \quad (\text{A.5})$$

By defining $\Lambda \equiv \frac{\partial \dot{\Gamma}}{\partial \Gamma}$ as the phase space *compression factor*, and integrating from $t = 0$ to $t = \tau$

$$f(\Gamma_t, t) = f(\Gamma_0, 0) \exp\left(-\int_0^\tau \Lambda dt\right). \quad (\text{A.6})$$

The compression factor for the infinitesimal phase space volume will be then given by

$$\frac{d\Gamma_\tau}{d\Gamma_0} = \exp\left(\int_0^\tau \Lambda dt'\right), \quad (\text{A.7})$$

since the probability of a specific phase space volume must be conserved.

A.1.2 Derivation of the FT via deterministic dynamics

Now we denote the evolution of a phase space point Γ for a certain time t using a time evolution operator U^t , and the time-reversal mapping operator R^T to the reverse trajectory, with is nothing but the trajectory with reverse momentum $p \rightarrow -p$. Then, a trajectory at Γ_0 has a corresponding anti-trajectory represented by $\Gamma_0^* \equiv R^T \Gamma_t = R^T U^\tau \Gamma_0$. Then, we obtain

$$d\Gamma_0^* = d\Gamma_\tau = d\Gamma_0 \exp\left(\int_0^\tau \Lambda dt\right). \quad (\text{A.8})$$

If we have a bundle of trajectories, the probability of observing an infinitesimal phase space volume $d\Gamma_0$ is

$$P(d\Gamma_0, 0) \equiv f(\Gamma_0, 0)d\Gamma_0. \quad (\text{A.9})$$

A system where the processes are described as macroscopically reversible must obey the condition of equal probabilities of observing the forward bundle of trajectories and the corresponding anti-trajectories, i.e.,

$$f(\Gamma_0, 0)d\Gamma_0 = f(\Gamma_0^*, 0)d\Gamma_0^*. \quad (\text{A.10})$$

In general, we can define a *dissipation function*, Ω_t to characterize the reversibility of the bundle of trajectories,

$$\Omega_\tau(\Gamma_0) \equiv \ln \left(\frac{P(d\Gamma_0, 0)}{P(d\Gamma_0^*, 0)} \right) = \ln \left(\frac{f(d\Gamma_0, 0)}{f(d\Gamma_0^*, 0)} \right) - \int_0^\tau \Lambda dt. \quad (\text{A.11})$$

In the case that the anti-trajectories are less probable, the dissipation function will be positive, and it will be negative otherwise. In the equilibrium state case, it takes the value 0. Also, this function has odd parity: $\Omega_\tau(\Gamma_0) = -\Omega_\tau(\Gamma_0^*)$.

By considering the entire phase space, we can calculate the probability of an anti-trajectory occurring by means of the relative probability of the dissipation function taking the opposite values, or

$$\frac{P(\Omega_t = A)}{P(\Omega_t = -A)} = \frac{\int d\Gamma_0 \delta(\Omega_\tau(\Gamma_0) - A) f(\Gamma_0, 0)}{\int d\Gamma_0^* \delta(\Omega_\tau(\Gamma_0^*) + A) f(\Gamma_0^*, 0)} \quad (\text{A.12})$$

$$= \frac{\int d\Gamma_0 \delta(\Omega_\tau(\Gamma_0) - A) f(\Gamma_0, 0)}{\int d\Gamma_0^* \delta(-\Omega_\tau(\Gamma_0) + A) f(\Gamma_0^*, 0)} \quad (\text{A.13})$$

$$= \frac{\int d\Gamma_0 \delta(\Omega_\tau(\Gamma_0) - A) f(\Gamma_0, 0)}{\int d\Gamma_0 \delta(-\Omega_\tau(\Gamma_0) + A) f(\Gamma_0, 0) \exp(-\Omega_\tau(\Gamma_0))} \quad (\text{A.14})$$

$$= \exp(A), \quad (\text{A.15})$$

where we used the parity of Ω_τ , Eq. (A.8), and the definition of the dissipation function. Therefore, we obtain the result of the FT described in Eq. (A.1), and the dissipation function is the so called entropy production. This FT means that, for all trajectories in the phase space, irreversible cases are exponentially more probable than the reversible ones. Furthermore, if we calculate the average of the dissipation

function over the whole phase space, we get

$$\begin{aligned}
\langle \exp(-\Omega_\tau) \rangle &= \int_{-\infty}^{\infty} dA \exp(-A) P(\Omega_t = A) \\
&= \int_{-\infty}^{\infty} dA \exp(A) P(-\Omega_t) \exp(A) \\
&= \int_{-\infty}^{\infty} dA P(\Omega_t = -A) \\
&= 1.
\end{aligned} \tag{A.16}$$

Moreover, this result implies exactly what it is expected from the second law inequality, i.e., $\langle \Omega_\tau \rangle \geq 0$.

A.2 The Crooks FT Fluctuation Theorem

As seen in the main text, the Crooks Fluctuation Theorem describes processes that start at a certain equilibrium state A, and after being removed from this state, it ends in a non-equilibrium state B. This process is denoted as *forward*, and its inverse, where the system evolves from a equilibrium state B to a non-equilibrium state A, is the *reverse* process. This FT reads

$$\frac{p_f(W = \mathcal{A})}{p_r(W = -\mathcal{A})} = \exp\left(\frac{\mathcal{A} - \Delta F}{k_B T}\right), \tag{A.17}$$

where $p_f(W = \mathcal{A})$ and $p_r(W = -\mathcal{A})$ are the probabilities of observing the forward and the reverse processes, respectively, $\Delta F = F_B - F_A$ is the free-energy change between the states A and B, k_B is the Boltzmann's constant, and T is the initial temperature of the system.

A.2.1 Introducing external work

If we want to introduce some external work by a control parameter λ , the Hamiltonian of the system will be given by

$$\mathcal{H}(\Gamma_t, t, \lambda_t) = \mathcal{T}(p) + \mathcal{V}(q, \lambda), \tag{A.18}$$

where \mathcal{T} and \mathcal{V} are the kinetic energy and the potential, respectively. The parameter λ varies from initial value $\lambda = A$ to the final value $\lambda = B$. The system before the introduction of the external work is in contact with a heat bath at a temperature T . Thus, this canonical ensemble can be described by the Boltzmann probability

distribution,

$$p(\mathcal{H}(\Gamma_0, A)) = \frac{e^{-\beta\mathcal{H}(\Gamma_0, A)}}{Z_A}, \quad (\text{A.19})$$

where $\beta = 1/k_B T$. After applying a protocol where λ varies from a initial value A to final value B, the final equilibrium state has the following probability distribution:

$$p(\mathcal{H}(\Gamma_\tau, B)) = \frac{e^{-\beta\mathcal{H}(\Gamma_\tau, B)}}{Z_B}. \quad (\text{A.20})$$

The Hamiltonian will also change, then we can write

$$\mathcal{H}(\Gamma_\tau, B) - \mathcal{H}(\Gamma_0, A) = W(\Gamma_0, \tau) + Q(\Gamma_0, \tau), \quad (\text{A.21})$$

where the total work done on the system is described by the first term, and the second one is the heat absorbed from the environment. These are also defined as

$$W(\Gamma_0, \tau) \equiv \int_0^\tau dt \frac{\partial \mathcal{H}(\Gamma, \lambda)}{\partial \lambda} \dot{\lambda} \quad (\text{A.22})$$

$$Q(\Gamma_0, \tau) \equiv \int_0^\tau dt \frac{\partial \mathcal{H}(\Gamma, \lambda)}{\partial \Gamma} \dot{\Gamma} = \beta^{-1} \int_0^\tau \Lambda(\Gamma_t) dt. \quad (\text{A.23})$$

In the Eq. (A.23) we directly apply a relation from the case in which heat slowly enters in a microcanonical ensemble, for states of equilibrium with quasi-static processes. In this scenario, the Boltzmann's entropy is defined as $S = k_B \log \zeta$, where ζ is the number of states. In a quasi-static process,

$$dS = \frac{dQ}{T}, \quad (\text{A.24})$$

then

$$\dot{Q} \equiv \frac{dQ}{dt} = T \frac{dS}{dt} = k_B T \frac{d}{dt} \log \zeta = k_B T \Lambda(\Gamma). \quad (\text{A.25})$$

Now, we can express the work done in terms of energy difference between the initial and final states, and the phase space compression factor,

$$W(\Gamma_0, \tau) = \mathcal{H}(\Gamma_\tau, B) - \mathcal{H}(\Gamma_0, A) - \beta^{-1} \int_0^\tau \Lambda(\Gamma_t) \quad (\text{A.26})$$

A.2.2 Derivation of the Crooks FT

After configuring our problem, we can finally structure the relationship between the probability distributions of the trajectories. Since the time evolution of this system is deterministic, the probability distribution associated with $W = \mathcal{A}$ is determined

by the initial function related to $\lambda = A$,

$$p_f(W = \mathcal{A}) = \int d\Gamma_0 \delta(W(\Gamma_0, \tau) - \mathcal{A}) p(\mathcal{H}(\Gamma_0, A)). \quad (\text{A.27})$$

Similarly, the probability distribution related to the anti-trajectories will be given by

$$p_r(W = -\mathcal{A}) = \int d\Gamma_0^* \delta(W(\Gamma_0^*, \tau) + \mathcal{A}) p(\mathcal{H}(\Gamma_0^*, B)). \quad (\text{A.28})$$

Finally, calculating the relative probability between the two processes, we get that

$$\frac{p_f(W = \mathcal{A})}{p_r(W = -\mathcal{A})} = \frac{\int d\Gamma_0 \delta(W(\Gamma_0, \tau) - \mathcal{A}) p(\mathcal{H}(\Gamma_0, A))}{\int d\Gamma_0^* \delta(W(\Gamma_0^*, \tau) + \mathcal{A}) p(\mathcal{H}(\Gamma_0^*, B))} \quad (\text{A.29})$$

$$= \frac{Z_B \int d\Gamma_0 \delta(W(\Gamma_0, \tau) - \mathcal{A}) e^{-\beta\mathcal{H}(\Gamma_0, A)}}{Z_A \int d\Gamma_0^* \delta(W(\Gamma_0^*, \tau) + \mathcal{A}) e^{-\beta\mathcal{H}(\Gamma_0^*, B)}} \quad (\text{A.30})$$

$$= \frac{Z_B \int d\Gamma_0 \delta(W(\Gamma_0, \tau) - \mathcal{A}) e^{-\beta\mathcal{H}(\Gamma_0, A)}}{Z_A \int d\Gamma_0 \delta(W(\Gamma_0, \tau) - \mathcal{A}) e^{-\beta\mathcal{H}(\Gamma_0, B)} e^{-\beta W(\Gamma_0, \tau)}} \quad (\text{A.31})$$

$$= \frac{Z_B}{Z_A} e^{\beta\mathcal{A}} \quad (\text{A.32})$$

$$= \exp(-\beta\Delta F + \beta\mathcal{A}). \quad (\text{A.33})$$

With some simplification, this result verifies the so called Crooks FT.

Appendix B

The Baker–Campbell–Hausdorff Formula

IN Quantum Mechanics, when we seek to obtain, for example, the temporal evolution of observables, relations often arise between matrix exponentials that do not necessarily commute. This type of calculus also appears with some frequency in Quantum Field Theory and Lie Theory, which in general is a special algebraic tool used in pure and applied mathematics. These are relations that do not behave like exponentials of numbers. In fact, in this case,

$$e^{A+B} \neq e^A e^B, \quad (\text{B.1})$$

where A and B can be any two non-commuting operators, i.e., $[A, B] \neq 0$. There is extensive literature that studies the properties of this relation [72, 136, 137]. However, a famous general formula derived from the Taylor expansion of exponentials can simplify our life in many cases when this type of exponential appears, and it is called the Baker-Campbell-Hausdorff (BCH) formula, named after Henry Frederick Baker, John Edward Campbell, and Felix Hausdorff have stated its qualitative form. It states that

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} e^{\frac{1}{3!}(2[B,[A,B]]+[A,[A,B]])} \dots \quad (\text{B.2})$$

When $[A, [A, B]] = 0$ and $[B, [A, B]] = 0$, this last expression results in

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}, \quad (\text{B.3})$$

where $[A, B] = c$, and it is just a number. Equation (B.3) is a special case when all higher order terms commute and the series truncates. If A and B commute, that is $[A, B] = 0$, the BCH formula reduces to $e^{A+B} = e^A e^B$.

Another very useful application of the BCH formula is when we have an operator between two exponentials. In this case we get that

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \dots \quad (\text{B.4})$$

This result can be obtained by expanding the "sandwich" on the left side and clustering terms of the same order. Beyond the third-order expansion, the calculations become cumbersome, thus we will only describe the BCH formula until this point.

Appendix C

Husimi Q function from the Wigner function

THE Wigner distribution was the first quasi-classical one, written from a wave function perspective. It is an interface between classical and quantum physics. Furthermore, distribution functions are an alternative but equivalent description of fluctuation phenomena that require the density operator. Originally, Wigner introduced its function in terms of the position and moment operators, and it has been widely used in a host of problems. However, for the sake of the development of this work, the coherent state's representation will be more suitable. This can be written in a general form as

$$W(\alpha, \alpha^*) = \frac{1}{\pi^2} \int \text{Tr}[\rho D(\beta)] e^{\alpha\beta^* - \alpha^*\beta} d^2\beta. \quad (\text{C.1})$$

where the displacement operator, $D(\beta) = e^{\beta a^\dagger - \beta^* a}$, can be rewritten, by using the BCH formula, as

$$D(\beta) = e^{\beta a^\dagger - \beta^* a} = e^{-\beta^* a} e^{\beta a^\dagger} e^{\frac{1}{2}|\beta|^2}. \quad (\text{C.2})$$

Thus, we have that

$$W(\alpha, \alpha^*) = \frac{1}{\pi^2} \int \text{Tr}[\rho e^{-\beta^* a} e^{\beta a^\dagger} e^{\frac{1}{2}|\beta|^2}] e^{\alpha\beta^* - \alpha^*\beta} d^2\beta. \quad (\text{C.3})$$

The trace has a cyclic property that establishes an invariance under cyclic permutations, what allows us to write

$$\text{Tr}[\rho e^{-\beta^* a} e^{\beta a^\dagger} e^{\frac{1}{2}|\beta|^2}] = e^{\frac{1}{2}|\beta|^2} \text{Tr}[e^{\beta a^\dagger} \rho e^{-\beta^* a}]. \quad (\text{C.4})$$

This trace can be evaluated in the integral form such as

$$\begin{aligned} \text{Tr}[e^{\beta a^\dagger} \rho e^{-\beta^* a}] &= \frac{1}{\pi} \int d^2\mu \langle \mu | e^{\beta a^\dagger} \rho e^{-\beta^* a} | \mu \rangle = \frac{1}{\pi} \int d^2\mu \langle \mu | e^{\beta \mu^*} \rho e^{-\beta^* \mu} | \mu \rangle \\ &= \frac{1}{\pi} \int d^2\mu e^{\beta \mu^*} e^{-\beta^* \mu} \langle \mu | \rho | \mu \rangle \end{aligned} \quad (\text{C.5})$$

This is also called "Gaussian filtering". By substituting this last relation in Eq. (C.3), we can write

$$\begin{aligned} W(\alpha, \alpha^*) &= \frac{1}{\pi^3} \int \int e^{\frac{1}{2}|\beta|^2} e^{\beta \mu^*} e^{-\beta^* \mu} \langle \mu | \rho | \mu \rangle e^{\alpha \beta^* - \alpha^* \beta} d^2\beta d^2\mu \\ &= \frac{1}{\pi^3} \int \int e^{\frac{1}{2}|\beta|^2} e^{(\alpha - \mu)\beta^* - (\alpha^* - \mu^*)\beta} \langle \mu | \rho | \mu \rangle d^2\beta d^2\mu. \end{aligned} \quad (\text{C.6})$$

The next step is achieved by completing the square

$$\frac{1}{2}|\beta|^2 + (\alpha - \mu)\beta^* - (\alpha^* - \mu^*)\beta = 2|\alpha - \mu|^2 + \frac{1}{2}(\beta + 2(\alpha - \mu))(\beta^* - 2(\alpha^* - \mu^*)). \quad (\text{C.7})$$

Therefore, we can simplify the Wigner function to

$$W(\alpha, \alpha^*) = \frac{2}{\pi^2} \int e^{2|\alpha - \mu|^2} \langle \mu | \rho | \mu \rangle d^2\mu. \quad (\text{C.8})$$

This last expression can be written in terms of a Husimi function of μ ,

$$W(\alpha, \alpha^*) = \frac{2}{\pi} \int e^{2|\alpha - \mu|^2} Q(\mu) d^2\mu, \quad (\text{C.9})$$

where

$$Q(\mu, \mu^*) = \frac{1}{\pi} \langle \mu | \rho | \mu \rangle. \quad (\text{C.10})$$

The Husimi Q-function can be described, as we can see, as the Weierstrass transform [138] of the Wigner function

$$Q(\mu, \mu^*) = \frac{2}{\pi} \int e^{-2|\mu - \alpha|^2} W(\alpha, \alpha^*) d^2\alpha. \quad (\text{C.11})$$

Appendix D

Examples

D.1 Coherent State

For the Husimi function of the coherent state $|\beta\rangle$ that characterizes the density matrix $\rho = |\beta\rangle\langle\beta|$,

$$Q(\alpha, \alpha^*) = \frac{1}{\pi} \langle\alpha|\rho|\alpha\rangle = \frac{1}{\pi} \exp(-|\alpha - \beta|^2), \quad (\text{D.1})$$

we have that the respective expectation values in relation (4.33) can be immediately obtained, and since $\langle J_\alpha J_{\alpha^*} \rangle = \langle J_\alpha \rangle = \langle J_{\alpha^*} \rangle = 0$, also the covariance between the two Husimi currents is zero. In the following calculation we give a direct proof.

Proof of $\langle J_\alpha J_{\alpha^*} \rangle = 0$.

$$\begin{aligned} \langle J_\alpha J_{\alpha^*} \rangle &= \int d^2\alpha Q(\alpha, \alpha^*) J_\alpha J_{\alpha^*} = \int d^2\alpha Q(-i\omega\alpha Q)(i\omega\alpha^* Q) \\ &= \omega^2 \int d^2\alpha |\alpha|^2 Q^3 = \omega^2 \int d^2\alpha |\alpha|^2 \left[\frac{1}{\pi} \exp(-|\alpha - \beta|^2) \right]^3 \\ &= \frac{\omega^2}{\pi^3} \int d^2\alpha |\alpha|^2 \exp(-3|\alpha - \beta|^2) \\ &= \frac{\omega^2}{\pi^3} \int d^2\alpha |\alpha|^2 \exp[-3(|\alpha|^2 + |\beta|^2 - \alpha\beta^* - \alpha^*\beta)] \end{aligned} \quad (\text{D.2})$$

In this last equation, the integral becomes

$$I = e^{-3|\beta|^2} \int_{-\infty}^{+\infty} d\alpha \alpha e^{3\alpha\beta^*} \int_{-\infty}^{+\infty} d\alpha^* \alpha^* e^{-3\alpha\alpha^* + 3\alpha^*\beta}. \quad (\text{D.3})$$

Solving for α^* first, we can write

$$I_{\alpha^*} = \int_{-\infty}^{+\infty} d\alpha^* \alpha^* e^{-3\alpha^*(\alpha - \beta)} = \int_{-\infty}^{+\infty} d\alpha^* \alpha^* e^{-3\alpha^*k}, \quad k \equiv \alpha - \beta, \quad (\text{D.4})$$

However, the direct calculation of this integral leads to a divergence. Thus, instead of doing this, we can make some modifications in order to obtain a convergence, such as defining

$$\alpha^* e^{-3\alpha^*k} = -\frac{1}{3k} \frac{\partial}{\partial \epsilon} [e^{-3\epsilon\alpha^*k}]_{\epsilon \rightarrow 1}, \quad (\text{D.5})$$

where ϵ is just a arbitrary variable. This will be useful for the rearrangement of the integral. Therefore, we have that

$$I_{\alpha^*} = -\frac{1}{3k} \frac{\partial}{\partial \epsilon} \int_{-\infty}^{\infty} e^{-3\epsilon\alpha^*k} d\alpha^* \quad (\text{D.6})$$

and $\epsilon \rightarrow 1$. Defining $t^2 = 3\epsilon\alpha^*k$, we have that $d\alpha^* = 2t dt/(3\epsilon k)$, and then

$$\int_{-\infty}^{\infty} e^{-3\epsilon\alpha^*k} d\alpha^* = \frac{2}{3\epsilon k} \int_{-\infty}^{\infty} t e^{-t^2} dt = 0. \quad (\text{D.7})$$

This integral results in zero since $t e^{-t^2}$ is an odd function and the interval $(-\infty, \infty)$ is symmetric about 0. Therefore, finally we have that $I_{\alpha^*} = 0$, and as consequence we can conclude that

$$\langle J_{\alpha} J_{\alpha^*} \rangle = 0. \quad (\text{D.8})$$

Proof of $\langle J_{\alpha} \rangle = 0$.

$$\begin{aligned} & \int d^2\alpha Q(\alpha, \alpha^*) J_{\alpha} = \int d^2\alpha Q(-i\omega\alpha Q) \\ &= -i\omega \int d^2\alpha \alpha Q^2 = -i\omega \int d^2\alpha \alpha \left[\frac{1}{\pi} \exp(-|\alpha - \beta|^2) \right]^2 \\ &= \frac{\omega}{i\pi^2} e^{-2|\beta|^2} \int d^2\alpha \alpha e^{-2|\alpha|^2} e^{2(\alpha\beta^* + \alpha^*\beta)} \\ &= \frac{\omega}{i\pi^2} e^{-2|\beta|^2} \int_{-\infty}^{\infty} d\alpha^* e^{2\alpha^*\beta} \int_{-\infty}^{\infty} d\alpha \alpha e^{-2|\alpha|^2 + 2\alpha\beta^*} \end{aligned} \quad (\text{D.9})$$

Solving for α first, by defining $m \equiv \alpha^* - \beta^*$, we have that

$$I_{\alpha} = \int_{-\infty}^{\infty} d\alpha \alpha e^{-2\alpha m} = -\frac{1}{2m} \frac{\partial}{\partial \epsilon} \left(\int_{-\infty}^{\infty} d\alpha e^{-2\alpha m \epsilon} \right)_{\epsilon \rightarrow 1}. \quad (\text{D.10})$$

The last integral can be written as

$$\int_{-\infty}^{\infty} d\alpha e^{-2\alpha m \epsilon} = \frac{1}{\epsilon m} \int_{-\infty}^{\infty} r e^{-r^2} dr, \quad (\text{D.11})$$

where $r^2 = 2\epsilon m \alpha$, and $d\alpha = (r/\epsilon m)dr$. For the same argument seen before, this integral is evaluated as zero. Therefore,

$$I_\alpha = 0 \quad \therefore \langle J_\alpha \rangle = 0. \quad (\text{D.12})$$

Proof of $\langle J_{\alpha^*} \rangle = 0$.

$$\begin{aligned} \langle J_{\alpha^*} \rangle &= \int d^2\alpha Q(\alpha, \alpha^*) J_{\alpha^*} = i\omega \int d^2\alpha \alpha^* Q^2 \\ &= i\omega \int d^2\alpha \alpha^* \left[\frac{1}{\pi} \exp(-|\alpha - \beta|^2) \right]^2 \\ &= \frac{i\omega}{\pi^2} e^{-2|\beta|^2} \int_{-\infty}^{\infty} d\alpha e^{2\alpha\beta^*} \int_{-\infty}^{\infty} d\alpha^* \alpha^* e^{-2|\alpha|^2 + 2\alpha^*\beta} \end{aligned} \quad (\text{D.13})$$

This calculation is similar to the previous one and also leads to a null result. Therefore, we will not cover it in its entirety in order not to overload the main text.

This covariance value means that there is no interdependence between the two currents in the numerical sense. In this case, for a Husimi function of a coherent state, we cannot establish a TUR by using the CRB. However, we can seek for solutions involving other types of functions based on different states, such as those computed in Chapter 3.

D.2 Fock State

For the Husimi function of the Fock state $|n\rangle$ that characterizes the density matrix $\rho = |n\rangle \langle n|$,

$$Q_n(\alpha, \alpha^*) = \frac{1}{\pi} \exp(-|\alpha|^2) \frac{(|\alpha|^2)^n}{n!}, \quad (\text{D.14})$$

we can set, for instance, $n = 1, 2$ in order to obtain

$$Q_1(\alpha, \alpha^*) = \frac{1}{\pi} \exp(-|\alpha|^2) |\alpha|^2, \quad (\text{D.15})$$

$$Q_2(\alpha, \alpha^*) = \frac{1}{\pi} \exp(-|\alpha|^2) \frac{(|\alpha|^2)^2}{2}. \quad (\text{D.16})$$

Applying this last two relations separately, we have that the expectation value for product between the Husimi currents will be given by

$$\begin{aligned}\langle J_\alpha J_{\alpha^*} \rangle_1 &= \omega^2 \int d^2\alpha |\alpha|^2 Q_1^3 = \omega^2 \int d^2\alpha |\alpha|^2 \left[\frac{|\alpha|^2}{\pi} \exp(-|\alpha|^2) \right]^3 \\ &= \frac{\omega^2}{\pi^3} \int d^2\alpha (|\alpha|^2)^4 \exp(-3|\alpha|^2), \quad (\text{for } n=1)\end{aligned}\tag{D.17}$$

and

$$\begin{aligned}\langle J_\alpha J_{\alpha^*} \rangle_2 &= \omega^2 \int d^2\alpha |\alpha|^2 Q_2^3 = \omega^2 \int d^2\alpha |\alpha|^2 \left[\frac{(|\alpha|^2)^2}{2\pi} \exp(-|\alpha|^2) \right]^3 \\ &= \frac{\omega^2}{8\pi^3} \int d^2\alpha (|\alpha|^2)^7 \exp(-3|\alpha|^2), \quad (\text{for } n=2).\end{aligned}\tag{D.18}$$

Solving for equation (D.17), we are going to follow a similar approach of that one of the previous section, but with minor modifications in the analysis of the integral. First, one can note that

$$\langle J_\alpha J_{\alpha^*} \rangle_1 = \frac{\omega^2}{\pi^3} \int d\alpha d\alpha^* (\alpha\alpha^*)^4 e^{-3\alpha\alpha^*} = \frac{\omega^2}{\pi^3} \int_{-\infty}^{\infty} \alpha^4 d\alpha \int_{-\infty}^{\infty} \alpha^{*4} e^{-3\alpha\alpha^*} d\alpha^*.\tag{D.19}$$

This last integral (for α^*) is an improper one and diverges as in the case of the coherent state. However, in order to get a convergence, we can apply the Cauchy Principal Value [139],

$$PV \int_{-\infty}^{\infty} f(x) dx \equiv \lim_{r \rightarrow \infty} \int_{-r}^r f(x) dx,\tag{D.20}$$

where $f(x)$ is an arbitrary function of some variable x . Then, we get

$$PV \int_{-\infty}^{\infty} \alpha^{*4} e^{-3\alpha\alpha^*} d\alpha^* = 0.\tag{D.21}$$

As consequence, also $\langle J_\alpha J_{\alpha^*} \rangle_1 = 0$. When we calculate the integral in Eq. (D.18), we also obtain that $\langle J_\alpha J_{\alpha^*} \rangle_2 = 0$. For the individual current averages, we will get

$$\begin{aligned}\langle J_\alpha \rangle_1 &= \frac{\omega}{i} \int d^2\alpha \alpha \left[\frac{1}{\pi} |\alpha|^2 e^{-|\alpha|^2} \right]^2 = \frac{\omega}{i\pi^2} \int d^2\alpha (\alpha\alpha^*)^2 \alpha e^{-2\alpha\alpha^*} \\ &= \frac{\omega}{i\pi^2} \int_{-\infty}^{\infty} \alpha^3 d\alpha \int_{-\infty}^{\infty} \alpha^{*2} e^{-2\alpha\alpha^*} d\alpha^*.\end{aligned}\tag{D.22}$$

By solving the integral from the right, we obtain a integral of kind

$$\int_{-\infty}^{\infty} \alpha^{*2} e^{-2\alpha\alpha^*} d\alpha^* = \frac{1}{4\alpha^3} \int_{-\infty}^{\infty} s^5 e^{-s^2} ds = 0, \quad (\text{D.23})$$

where we set $s^2 = 2\alpha\alpha^*$ and $d\alpha^* = (t/\alpha)dt$. Therefore, for the current J_{α^*} , we also get $\langle J_{\alpha^*} \rangle = 0$, and the covariance of the currents for $|1\rangle$ is zero. For the Fock state $|2\rangle$ we have similar calculations, and then $\Delta(J_{\alpha}, J_{\alpha^*}) = 0$ for both cases. Interestingly, it is noted that for both odd and even numbers in $|n\rangle$, we have obtained similar results, always with some integral of the type (D.23) being found.

D.3 Thermal State

For the Husimi function of the thermal state in Eq. (3.76),

$$Q_T(\alpha, \alpha^*) = \frac{(1 - e^{-\hbar\omega/k_B T})}{\pi} \exp[-|\alpha|^2 (1 - e^{-\hbar\omega/k_B T})], \quad (\text{D.24})$$

or, defining $\mathcal{B} = e^{-\hbar\omega/k_B T}$, the calculation for the averages leads to

$$\begin{aligned} \langle J_{\alpha} J_{\alpha^*} \rangle_T &= \omega^2 \int d^2\alpha |\alpha|^2 Q_T^3 = \omega^2 \int d^2\alpha |\alpha|^2 \left[\frac{(1 - \mathcal{B})}{\pi} e^{-|\alpha|^2(1 - \mathcal{B})} \right]^3 \\ &= \frac{\omega^2}{\pi^3} (1 - \mathcal{B})^3 \int d^2\alpha |\alpha|^2 e^{-3|\alpha|^2(1 - \mathcal{B})}. \end{aligned} \quad (\text{D.25})$$

However, if we set $\alpha(1 - \mathcal{B}) = k$, the integral for α^* becomes similar to that one in Eq. (D.4), what gives us the same result of Eq. (D.8), i.e., $\langle J_{\alpha} J_{\alpha^*} \rangle = 0$. Now, for $\langle J_{\alpha} \rangle$ and $\langle J_{\alpha^*} \rangle$, we have that

$$\langle J_{\alpha} \rangle_T = \frac{\omega}{i} \int d^2\alpha \alpha \left[\frac{(1 - \mathcal{B})}{\pi} e^{-|\alpha|^2(1 - \mathcal{B})} \right]^2 = \frac{\omega(1 - \mathcal{B})^2}{i\pi^2} \int d^2\alpha \alpha e^{-2|\alpha|^2(1 - \mathcal{B})}. \quad (\text{D.26})$$

By setting $\alpha^*(1 - \mathcal{B}) = m$, we obtain a integral similar to (D.10), and then

$$\langle J_{\alpha} \rangle_T = 0 \quad \therefore \quad \Delta(J_{\alpha}, J_{\alpha^*})_T = 0. \quad (\text{D.27})$$

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