UNIVERSIDADE FEDERAL DO PARANÁ

JOSÉ CARLOS LIBOIS NETO

TIME IN QUANTUM MECHANICS: CONSIDERATIONS ON QUANTIZATION AND CORRELATIONS

CURITIBA

2025

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Dissertação apresentada ao Programa de Pós-Graduação em Física, no Setor de Ciências Exatas, na Universidade Federal do Paraná, como requisito parcial para a obtenção do título de Mestre em Física.

Supervisor: Prof. Dr. Renato Moreira Angelo

CURITIBA

2025

DADOS INTERNACIONAIS DE CATALOGAÇÃO NA PUBLICAÇÃO (CIP)
UNIVERSIDADE FEDERAL DO PARANÁ
SISTEMA DE BIBLIOTECAS – BIBLIOTECA CIÊNCIA E TECNOLOGIA

Libois Neto, José Carlos
Time in quantum mechanics: considerations on quantization and correlations. / José Carlos Libois Neto. – Curitiba, 2025.
1 recurso on-line : PDF.

Dissertação (Mestrado) - Universidade Federal do Paraná, Setor de Ciências Exatas. Programa de Pós-Graduação em Física.

Orientador: Prof. Dr. Renato Moreira Angelo

1. Mecânica quântica. 2. Tempo. 3. Realismo. I. Universidade Federal do Paraná. II. Programa de Pós-Graduação em Física. III. Angelo, Renato Moreira. IV. Título.

Bibliotecária: Roseny Rivelini Morciani CRB-9/1585

TERMO DE APROVAÇÃO

Os membros da Banca Examinadora designada pelo Colegiado do Programa de Pós-Graduação FÍSICA da Universidade Federal do Paraná foram convocados para realizar a arguição da Dissertação de Mestrado de **JOSÉ CARLOS LIBOIS NETO**, intitulada: **"Time in Quantum Mechanics: Considerations on Quantization and Correlations"**, sob orientação do Prof. Dr. RENATO MOREIRA ANGELO, que após terem inquirido o aluno e realizada a avaliação do trabalho, são de parecer pela sua APROVAÇÃO no rito de defesa.
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CURITIBA, 26 de Fevereiro de 2025.

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AGRADECIMENTOS

Agradeço à minha mãe e à minha irmã pelos momentos bons e pelos momentos difíceis.

Agradeço aos colegas que fiz nesta instituição e dos quais nunca me esquecerei.

Agradeço à Prof.ª Ana S. Costa e ao Prof. Milton M. Fujimoto pela revisão e pelos comentários.

Agradeço ao Prof. Marcus W. Beims e ao Prof. Fabiano M. Andrade por aceitarem participar da minha banca de defesa.

Agradeço à CAPES pelo auxílio financeiro.

Agradeço, em especial, ao meu orientador, Prof. Renato M. Angelo. A maior qualidade de um educador não é apenas a bagagem intelectual, mas sim a paciência.

"Life is what happens when you are making other plans."
John Lennon

RESUMO

O tempo é uma das grandezas mais estudadas pela humanidade, mas também uma das mais enigmáticas. Na maior parte da Física, ele é tratado como um parâmetro que mede a evolução de sistemas dinâmicos, e seu papel na mecânica quântica não foge a essa abordagem. O objetivo deste trabalho é investigar a natureza do tempo dentro da mecânica quântica, com o propósito de fornecer uma visão mais abrangente sobre esse tema fundamental. Esta dissertação se concentra em duas principais linhas de investigação. Na primeira, exploramos a possibilidade de tratar o tempo como um observável. Para isso, analisamos a abordagem do operador de Aharonov-Bohm e o mecanismo de Page-Wootters, avaliando a aplicabilidade de seus estados temporais como marcadores de caminho em interferômetros quânticos. A partir dessa análise, discutimos se o tempo pode, de fato, ser considerado um observável. Na segunda linha de investigação, estudamos as correlações temporais. Abordamos o paradoxo de Einstein-Podolsky-Rosen, o Teorema de Bell e o irrealismo de Bilobran-Angelo, e posteriormente analisamos as correlações temporais no contexto do macrorealismo de Leggett-Garg. Como contribuição original, propomos um quantificador de multi-irrealismo, estendemos essa ferramenta para observáveis dinâmicos e comparamos sua eficácia com um quantificador de correlações de Leggett-Garg.

Plavras-chaves: Operador tempo; irrealismo; macrorealismo; correlações.

ABSTRACT

Time is one of the most studied quantities by humanity, yet it remains one of the most mysterious. In most of physics, time is treated merely as a parameter that measures changes in dynamical systems. In quantum mechanics, its treatment is identical. The objective of this work is to investigate the concept of time within quantum theory, with the aim of providing a more comprehensive understanding of this highly relevant topic within one of the greatest theories of physics. This work addresses two main lines of investigation. In the first, we discuss the possibility of treating time as an observable. To this end, we explore the Aharonov-Bohm operator approach and the Page-Wootters mechanism, and we propose the applicability of their temporal states as path markers in quantum interferometers, arguing whether time is an observable or not. In the second part, we address temporal correlations. For this, we discuss the Einstein-Podolsky-Rosen paradox, Bell's theorem, and the Bilobran-Angelo irrealism. Subsequently, we examine temporal correlations in the context of Leggett-Garg macrorealism. We also propose the existence of a multi-irrealism quantifier, extend this tool to dynamical observables, and compare this new tool with a Leggett-Garg correlation quantifier.

Key-words: Time operator; irrealism; macrorealism; correlations.

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CHAPTER 1

Introduction

A cornerstone in the philosophy of science is "The Structure of Scientific Revolutions" [1], by Thomas Kuhn, in which he describes how science has developed throughout human history. In this seminal book, the author defines the concept of *paradigms*, which are a set of practices, theories, methods, and standards shared by a scientific community that define legitimate work in a field, such as the Newtonian mechanics or the theory of electromagnetism.

After the establishment of new paradigms, the period of *normal science* begins, during which scientists work within these paradigms, solving problems using established methods. However, some *anomalies* arise in theoretical discussions or experiments and cannot be explained by the paradigms. Initially, these anomalies are often ignored or treated as errors. When they start to accumulate and resist solutions, the scientific community enters in a period of *crisis*. This crisis paves the way for the development of new paradigms that can better explain experimental results and theoretical conflicts. The combination of these new paradigms leads to the development of new theories, marking the beginning of a *scientific revolution*.

The scientific community was in a period of crisis in the early 20th century, which marked the beginning of a scientific revolution known as the *Einsteinian revolution*. During this period, a significant number of anomalies were observed, one of the most intriguing being the double-slit experiment with matter performed in 1927 by Davisson and Germer [2] and independently by George Paget Thomson and his assistant Alexander Reid [3]. In the original version of the experiment performed in 1804, Thomas Young positioned a double-slit apparatus in front of a film [4]. By directing a light beam toward the apparatus, he observed on the film an interference pattern, indicating that light exhibits wave like behavior. Decades later, this experiment was extended to electrons, and experimentalists observed the same interference pattern that Young had described. This result was unexpected, as particles were not thought to exhibit self-interference. Furthermore, any attempt to determine which slit the particle passed through resulted in the destruction of the interference pattern. (A variation of this experiment will be revisited in Chapter 3.)

This anomaly indicated that physicists needed to propose new paradigms. They posited that, in the microscopic world, a physical system is described by wave functions, which can interfere with themselves and possess a probabilistic interpretation. Furthermore, they established that upon any measurement, the wave function collapses into a unique state, and that the act of measurement introduces uncertainty. Specifically, the precision in determining the slit through which a particle passes disrupts the interference pattern. These new paradigms, along with many others, collectively formed what is now known as the theory of quantum mechanics.

Despite quantum mechanics being one of the most prolific scientific theories in human history, capable of predicting phenomena and effects previously unknown, many physicists criticized its fundamentally probabilistic interpretation of nature. Among many critical works, one of the most influential was authored by Einstein, Podolsky, and Rosen (EPR), entitled “Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?” [5]. In this paper, the authors introduce the concept of elements of reality, which states that if it is possible to determine the value of a physical quantity with probability equal to unity, then this quantity represents an element of reality. They further define that a theory is considered complete if every element of reality has a corresponding counterpart in the theory.

For example, if the position of a particle is well defined, then the position represents a element of reality. But, it is a well known fact that two incompatible observables, such as position and momentum, cannot be measured simultaneously with arbitrary uncertainty. This means that, in this example, while the position is an element of reality, the momentum is not. Consequently, they proposed two alternatives: either quantum mechanics is an incomplete theory, or it is impossible for two incompatible physical quantities to simultaneously represent elements of reality. Using a thought experiment, they argue that the second alternative is possible, leading them to conclude that quantum mechanics must be incomplete.

In response to the EPR paper, Niels Bohr published the homonymous article “Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?” [6]. In this work, Bohr argues that it is not possible to determine whether a physical quantity represents an element of reality prior to measurement. This implies that physical quantities are not well-defined before the experimental procedure. Regarding the discussion on the completeness of quantum mechanics, Bohr contends that the EPR argument attempts to simultaneously address two complementary physical quantities, which is prohibited by the principle of complementarity.

The EPR paper sparked heated debates within the scientific community regarding the completeness of quantum mechanics in describing reality. One possibility that emerged was the supplementation of *hidden variables* into quantum mechanics [7], aiming to restore its deterministic nature. The notion of determinism is closely tied to the concept of realism. A system satisfies realism if it is possible to determine a physical quantity with infinite precision without disturbing the system [8]. The EPR paper specifically adopted the notion of local realism, where the reality of a physical quantity is well-defined and cannot be influenced by actions performed at a distance.

Inspired by the debate initiated by EPR and Bohr, Bell demonstrated that any theory of local hidden variables is incompatible with quantum mechanics [9]. This result implies that quantum mechanics is a complete theory but not a local one, contrary to what EPR had proposed. A few years later, Clauser, Horne, Shimony, and Holt (CHSH) refined Bell's work and introduced the CHSH inequality [10], which served the same purpose as Bell's theorem but was better suited for experimental verification.

Many works on realism were published following the EPR paper. Leggett and Garg [11], inspired by the CHSH inequality, proposed a similar inequality; however, instead of using different observables, they considered a single dynamical observable evaluated at different instants of time. They defined certain assumptions about how macroscopic systems should behave. If a system does not adhere to these assumptions, their inequality is violated. In a separate discussion, Bilobran and Angelo (BA) redefined the concept of elements of reality and proposed an irreality quantifier, which can be used to determine whether a physical quantity represents an element of reality in the BA framework or not [12]. Both topics will be discussed in details in Chapter 4.

Until now, we have discussed the problems of locality and determinism in quantum mechanics. But there is a different problem, which is not as discussed as the other two: time. Time is one of the most fundamental concepts in physics, but yet not properly defined. In most cases, the treatment of time in quantum mechanics is the same as in classical mechanics, it is a parameter that represents changes in a physical system. In fact, a parameter in physics is a scalar, variable or constant, that is sharply defined for any kind of measurement made in a system, such as mass, charge or time. An unique application of the parameter time in quantum mechanics is seen in the time-energy uncertainty relation, where it is possible to define the time scale over which a system undergoes significant changes. A different approach to the same concept is seen in the Mandelstam-Tamm uncertainty relation, which will be derived and interpreted in chapter 3.

Another interesting discussion about time in physics is the arrow of time, which state that time is asymmetric, i.e. time flows in only one direction and the cause comes before the consequence. The direction of the time flow is expressed by the second law of thermodynamics, which states that the entropy of closed systems tend to increase with time. In quantum mechanics, the arrow of time states that future observations made on a system do not interfere with previous one, meaning that the collapse of the wave function cannot interfere with the preparation of a system.

In the time-energy uncertainty principle and the arrow of time, time is treated as a parameter. But this kind of time is not seen in another great physical theory, the general relativity. In general relativity, space and time are unified into a single four-dimensional continuum called spacetime. But in quantum mechanics, only space is treated as a physical quantity, with its unique operator, and can be measured, while time is treated as a parameter and it is measured indirectly by the evolution of a system. This suggests that, if quantum mechanics and relativity are consistent with each other, than time should also be treated as a physical quantity.

In the past few decades, more and more physicists have seen the quantization of time as a path to the development of quantum gravity, making it a more relevant topic. One of the first problems with the quantization of time was stated by Pauli [13]. He says that a self-adjoint operator and a bounded Hamiltonian cannot satisfy the canonical commutation relation. This is called the Pauli objection. Aharonov and Bohm constructed a time operator that satisfy this objection [14], while Page and Wootters bypass it by using external quantum clocks [15]. Furthermore, in the formalism proposed by Dias and Parisio, the authors treats time equivalently as space, resulting in the time probability for a quantum state to collapse [16]. More recently, Arlans and Beims presented an approach to treat the quantization of time that allows for predicting times of flight and tunneling times in a spacetime-symmetric extension of non-relativistic quantum mechanics [17]. Some of this topics will be discussed in chapter 4.

Our objective in this work it to create a complete discussion about time in quantum mechanics, approaching the concept of time observable and time correlations. The question that we want to answer in the first part of our work is, if time is indeed a physical quantity with a proper operator acting on a Hilbert space, then different time of flights in interferometers can be used to create which way information? To do so, we will show how which way information is created and also a possible experiment to test this hypothesis. In the second part, we will discuss time correlations in quantum systems, first revising the concept in the macrorealism scenario, and then developing a irreality quantifier for different times and compare it numerically with a macrorealism quantifier.

This work is divided as follows: In Chapter 2, we will introduce important physical concepts and mathematical tools that will be used throughout this work. In Chapter 3, we will discuss the possibility of use different time of flights as which way information. To do so, we will show two approaches of time observables in the literature: the Aharonov-Bohm time operator and the Page-Wootters mechanism. After this, we will revise the complementary principle and show how which way information is created in interferometers. With this, we discuss the hypothesis of time as which way information and show a possible experiment to prove the hypothesis. In Chapter 4, we will discuss the concept of time correlations. First, we need to understand the EPR paradox and how Bell showed the impossibility of local realism in quantum mechanics. We will also explore the concept of the irreality quantifier, which underpins the discussion in the EPR paper. Following this, we will revise the concept of macrorealism, which defines how macroscopic objects should behave. In the final section, we will introduce a new irreality quantifier called multi-irreality, extend this mathematical tool for dynamical observables and compare it with a quantifier of the Leggett-Garg correlator.

CHAPTER 2

Theoretical Foundations of Quantum Mechanics

2.1 Stern-Gerlach Experiment

The Stern-Gerlach (SG) experiment was first introduced by Otto Stern in 1921 and later reproduced by him and Walther Gerlach in 1922 [18]. This experiment was able to demonstrate not only the existence of a new physical quantity called *spin*, but also to clarify several fundamental concepts of quantum mechanics that were being discussed and theorized by physicists at the time.

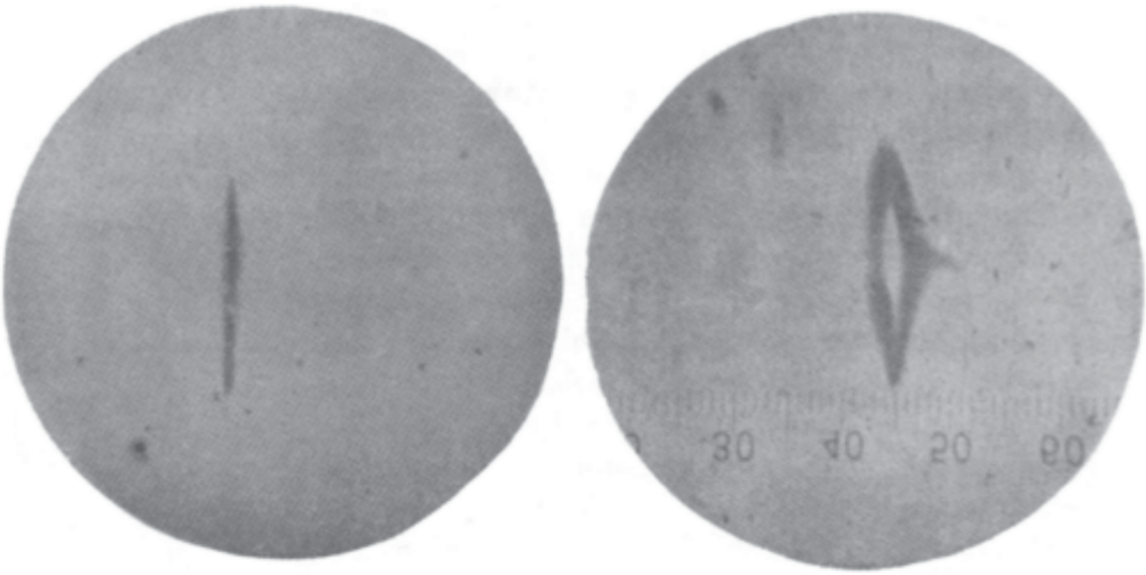
The experiment proceeds as follows: First, silver atoms are heated in an oven with a small hole in its surface. The atoms are then collimated into a beam and subjected to an inhomogeneous magnetic field, known as the SG apparatus. After passing through the magnetic field, the atoms collapse on a glass plate, where the force exerted on the particles by the field can be inferred from the distance between the end of the magnetic field and the points on the plate where the atoms are collapsed.

Classically, the deflection of the atom's trajectory is caused by the force associated with the interaction between the magnetic field $\vec{B}$ and the magnetic moment of the silver atoms $\vec{\mu}$:

$$F_z = \frac{\partial}{\partial_z}(\vec{B} \cdot \vec{\mu}) \approx \mu_z \frac{\partial B_z}{\partial z}, \tag{2.1}$$

where it is assumed that the magnetic moment $\vec{\mu}$ is homogeneous and it is taken into account only the z component of the magnetic field and the force experienced by the atom.

In the first case, without a magnetic field, the particle did not experience any



(a) (b)

Figure 1 – The plates of the Stern-Gerlach experiment. In (a) there is no external magnetic field, and the collapse of the atoms form a line. In (b) there is a inhomogeneous magnetic field, and the collapse of the atoms split in two lines. Picture taken from [18].

deflection in its trajectory since the force is null. As a result, the image on the plate after passing through the apparatus was a line parallel to the direction of the field, caused by the various possible trajectories of the particle. In the second case, an inhomogeneous magnetic field is applied. The physicists expected the result to be the same as in the first case, since the atomic theory of that time did not predict a magnetic moment for the atom. However, instead of a line, they observed a split of the line on the plate: one above and one below the center (Figure 1).

The fact that the atoms were deflected in the presence of an inhomogeneous magnetic field was in complete disagreement with the physics of that time. First, atoms were not expected to have an intrinsic magnetic moment, and second, since only two lines were observed on the plate after passing through the apparatus, the intrinsic magnetic moment of atoms could only have two possible values in the direction of the magnetic field.

To solve this problem, it was proposed that electrons had an intrinsic magnetic moment called spin. In the case of silver atoms, which have 47 electrons in their structure, the net spin of the atom is equal to the spin of the unpaired electron. Not only that, but it was also proposed that the spin component in the direction of the field can only have two values: $\hbar/2$ and $-\hbar/2$, where these values were determined by the length of the deflections observed in the experiment, and $\hbar = h/2\pi$ is the reduced Planck constant. The positive value of spin is observed when the atom is in the $S_z;+$

configuration, and the negative value is observed when it is in the $S_z; -$ configuration.

2.1.1 Sequential Stern-Gerlach Experiment

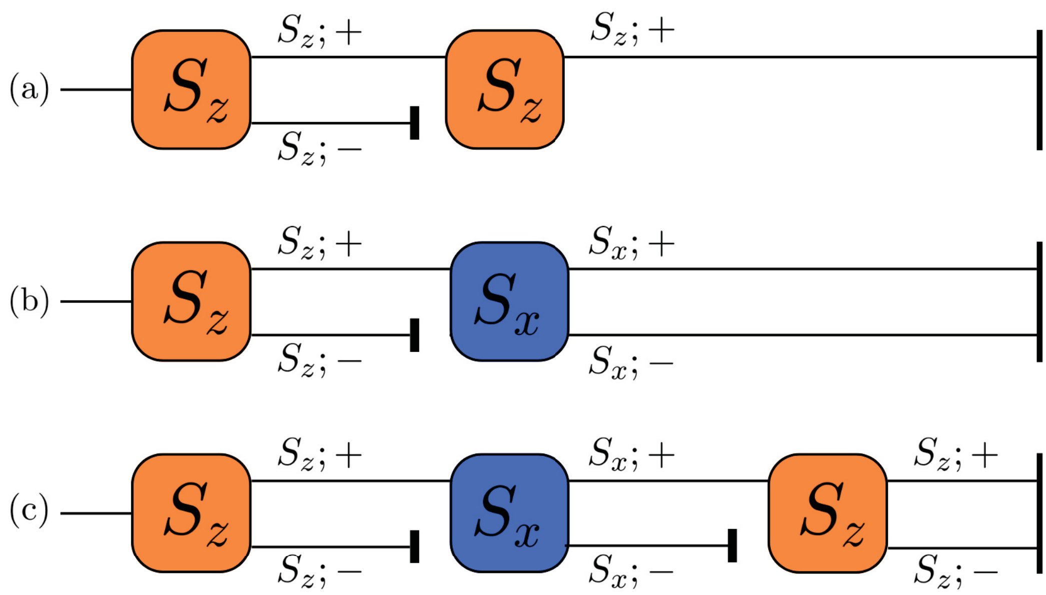


Figure 2 – Diagram of the sequential SG experiment. In (a), a beam of atoms is polarized, selecting those with the $S_z; +$ configuration, and is polarized again in the same direction, resulting in a beam with the same configuration. In (b), the first step is repeated, followed by polarization in the S_x direction, starting with the beam in the $S_z; +$ configuration. This produces two beams, each with one of the two possible configurations. In (c), both steps from the previous case are repeated, followed by polarization in the S_z direction with the beam in the $S_x; +$ configuration, resulting in two beams, each with one of the two possible configurations.

Having introduced the SG experiment, we now present the sequential SG experiment [19], as illustrated in Figure 2. In case (a), a similar experiment to the one in the previous section is performed, but the atoms with the $S_z; -$ configuration are blocked. This results in a polarized beam of atoms in the $S_z; +$ configuration. Subsequently, another SG apparatus is used, aligned in the same direction. As expected, the beam maintains the $S_z; +$ configuration.

In case (b), the same polarized beam of atoms in the $S_z; +$ configuration is used. However, in the second interaction, a SG apparatus aligned along the orthogonal direction (the x-axis) is employed. The observation reveals two emerging beams from the apparatus. This result is unexpected, as the initial beam was polarized in the $S_z; +$ configuration, yet two beams with the $S_x; +$ and $S_x; -$ configurations are now present. This outcome challenges the initial assumption that the polarized beam would not interact with the second apparatus in this manner, prompting a reevaluation of the notion that spin behaves as an intrinsic magnetic moment similar to that in classical electromagnetism.

In case (c), the same configuration as in the previous experiment is repeated, but the $S_x; -$ beam is blocked, leaving only atoms with the $S_x; +$ configuration. This beam is then directed into an SG apparatus aligned along the z-axis. The observation reveals that the beam splits into two paths. Given that the atoms were previously polarized, it is puzzling that they now exhibit two possible spin configurations along the z-axis. This suggests that sequential polarization of spin in orthogonal directions may erase prior information about the spin state. A more detailed discussion of this experiment will follow in subsequent sections.

2.2 Postulates of Quantum Mechanics

There are multiple ways to discuss the fundamentals of quantum mechanics. In this work, we apply a unique approach, in which we define the postulates of quantum mechanics as presented in [20], with minor modifications accompanied by necessary comments. We will also present the applications of these postulates in the SG experiment previously discussed in the last section. The first postulate goes as follows:

Postulate 1: At a fixed time t_0, the state of an isolated physical system is defined by specifying a ket $|\psi(t_0)\rangle$ belonging to the state space $\mathcal{H}$.

Hilbert spaces $\mathcal{H}$ are complex vector spaces. The elements of this space are represented as state vectors, written as kets $|\psi\rangle$ in the Dirac notation [21], along with their dual counterparts, the bra states $\langle\psi|$. The Hilbert space is equipped with an inner product, denoted as $\langle\psi|\psi\rangle$. The norm of a state is defined as $\| \, |\psi\rangle \, \| = \sqrt{\langle\psi|\psi\rangle}$.

Given that a linear combination of states also constitutes a valid state, it follows that a system can exist in more than one state simultaneously. This phenomenon is described by the *superposition principle*. By the result observed in the SG experiment in (a), the state of the system in an instant t_0 previous to any observation is expressed as $|\psi(t_0)\rangle = \frac{1}{\sqrt{2}}(|+, z\rangle + |-, z\rangle)$, where $|+, z\rangle$ represents atoms with the $S_z; +$ configuration, and $|-, z\rangle$ represents atoms with the $S_z; -$ configuration. The constant $\frac{1}{\sqrt{2}}$ is chosen to ensure that the state $|\psi(t_0)\rangle$ is properly normalized ($\| \, |\psi\rangle \, \| = 1$).

Composite system postulate: The Hilbert space of a composite system is the Hilbert space tensor product of the state spaces associated with the component systems. For a non-relativistic system consisting of a finite number of distinguishable particles, the component systems are the individual particles.

For two atoms, A and B, interacting with each other, with theirs respective Hilbert spaces $\mathcal{H}_A = \{|a_n\rangle\}$ and $\mathcal{H}_B = \{|b_m\rangle\}$, the total Hilbert space of the system is given by $\mathcal{H}_T = \mathcal{H}_A \otimes \mathcal{H}_B = \{|a_n\rangle \otimes |b_m\rangle\}$. A general state in the space $\mathcal{H}_T$ is

$$|\psi\rangle = \sum_{n,m} c_{nm} |a_n\rangle \otimes |b_m\rangle . \tag{2.2}$$

The state $|\psi\rangle$ is entangled if the states are not separable, i.e. $c_{nm} \neq c_n c_m$. An example of an entangled state for spin systems is the singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+,z\rangle_A |-,z\rangle_B - |-,z\rangle_A |+,z\rangle_B). \tag{2.3}$$

Since the state $|\psi\rangle$ cannot be expressed as a product state, the state is entangled.

In the case of composite systems, it is also necessary to redefine the operators acting on the subsystems. Given operators $A : \mathcal{H}_A \to \mathcal{H}_A$ and $B : \mathcal{H}_B \to \mathcal{H}_B$, the corresponding operators for the composite space are $A \otimes \mathbb{1}_B : \mathcal{H}_T \to \mathcal{H}_T$ and $\mathbb{1}_A \otimes B : \mathcal{H}_T \to \mathcal{H}_T$, where $\mathbb{1}_A$ and $\mathbb{1}_B$ denote the identity operators on the spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively

Postulate 2.a: Every measurable physical quantity $\mathcal{A}$ is described by a Hermitian operator A acting in the state space $\mathcal{H}$. This operator is an observable, meaning that its eigenstates form a basis for $\mathcal{H}$. The result of measuring a physical quantity $\mathcal{A}$ must be one of the eigenvalues of the corresponding observable $\mathcal{A}$.

All operators associated with physical quantities need to be Hermitian ($A = A^\dagger$), otherwise their eigenvalues could be complex. Operators can be written by their spectral decomposition

$$A = \sum_n a_n |a_n\rangle \langle a_n| = \sum_n a_n \Lambda_{a_n}, \tag{2.4}$$

where $|a_n\rangle$ are the eigenstates of A and a_n their respective eigenvalue. The contractions Λ_{a_n} are called projection operators, or simply projectors, and they satisfy the completeness relation ($\sum_n \Lambda_{a_n} = 1$) and pairwise orthogonality ($\Lambda_{a_n}\Lambda_{a_m} = \Lambda_{a_n}\delta_{nm}$).

In the SG experiment, the possible outcomes of a measurement are $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$. Then, the operator associated with the spin in the z-direction S_z is

$$S_z = \frac{\hbar}{2} |+,z\rangle \langle +,z| - \frac{\hbar}{2} |-,z\rangle \langle -,z| . \tag{2.5}$$

An important tool we will use in this work is the trace of an operator. For an operator A, its trace is given by

$$\mathrm{Tr}[A] = \sum_n \langle a_n| A |a_n\rangle , \tag{2.6}$$

which is the sum of the diagonal elements of A.

Postulate 2.b: When the physical quantity $\mathcal{A}$ is measured on a system in a normalized state $|\psi\rangle$, the probability of obtaining an eigenvalue of the corresponding observable A is given by the amplitude squared of the appropriate wave function (projection onto corresponding eigenstate):

$$P(a_n) = |\langle a_n|\psi\rangle|^2. \tag{2.7}$$

Given that the state of a spin system is

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+,z\rangle + |-,z\rangle), \tag{2.8}$$

the probability of observing one of the two possible outcomes is

$$P_z(+) = |\langle +,z|\psi\rangle|^2 = \frac{1}{2}, \qquad P_z(-) = |\langle -,z|\psi\rangle|^2 = \frac{1}{2}, \tag{2.9}$$

which is exactly what is observed in the SG experiment.

Another important quantity is the expectation value, generally defined as $\langle\psi| A |\psi\rangle = \mathrm{Tr}[A\rho] = \langle A\rangle$. Similarly to the expectation values in probability theory, this quantity represents the average of all possible outcomes weighted by their respective probabilities. For the state in (2.8), the expectation value $\langle S_z\rangle$ is

$$\langle S_z\rangle = \langle\psi| \left(\frac{\hbar}{2}|+,z\rangle\langle +,z| - \frac{\hbar}{2}|-,z\rangle\langle -,z|\right)|\psi\rangle \tag{2.10}$$

or

$$\langle S_z\rangle = \frac{\hbar}{2}\left(|\langle +,z|\psi\rangle|^2 - |\langle -,z|\psi\rangle|^2\right) = 0 \tag{2.11}$$

The result $\langle S_z\rangle = 0$ means that all possible outcomes have the same probability of being observed.

Postulate 2.c: If the measurement of the physical quantity $\mathcal{A}$ on the system in the state $|\psi\rangle$ gives the result a_n, then the state of the system immediately after the measurement is the normalized projection of $|\psi\rangle$ onto the eigensubspace associated with a_n:

$$|\psi'\rangle = \frac{\Lambda_{a_n}|\psi\rangle}{\sqrt{\langle\psi|\Lambda_{a_n}|\psi\rangle}}. \tag{2.12}$$

Given the experiment in Figure 2, in case (a), the state after the first selective measurement is

$$|\psi'\rangle = \frac{\Lambda_{z,+}|\psi\rangle}{\sqrt{\langle\psi|\Lambda_{z,+}|\psi\rangle}} = |z,+\rangle, \tag{2.13}$$

where $\Lambda_{z,+} = |z,+\rangle \langle z,+|$. The expectation value of the observable S_z after the second measurement is $\langle \psi'| S_z |\psi'\rangle = 1$. This result is expected, as the system has already been measured, and its state is known with certainty.

In case (b), the projected state remains $|\psi'\rangle = |z,+\rangle$. However, a measurement of the observable S_x is now performed. The apparatus yields two possible outcomes, indicating that the state $|z,+\rangle$ can be expressed as a superposition of the eigenstates of S_x:

$$|z,+\rangle = \frac{1}{\sqrt{2}}(|x,+\rangle + |x,-\rangle), \tag{2.14}$$

and since $|z,+\rangle$ and $|z,-\rangle$ must be orthogonal,

$$|z,-\rangle = \frac{1}{\sqrt{2}}(|x,+\rangle - |x,-\rangle). \tag{2.15}$$

In case (c), a measurement of the observable S_z is performed for the system in the state $|x,+\rangle$. The expectation value for this state is $\langle S_z\rangle = 0$, which is consistent with the experimental observations.

The result of the experiment is counterintuitive from the perspective of classical physics. Although a projective measurement of the observable S_z has been performed, the information about the spin in that direction is not preserved. This implies that the measurement of one observable erases all prior information about another incompatible observable. In other words, it is impossible to simultaneously determine the precise values of two incompatible observables. Two observables are said to be incompatible when

$$[A, B] = AB - BA \neq 0, \tag{2.16}$$

where $[A, B]$ is called commutator. A more intuitive way to look at this is through the uncertainty relation. For any two observables A and B, the product of their uncertainties must satisfy the inequality

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A, B]\rangle|^2. \tag{2.17}$$

where $\langle(\Delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$ is referred to as the dispersion of the observable A. This quantity represents the uncertainty associated with the physical quantity for a given state. For the state $|+, z\rangle$, the dispersion of the observable S_z is $\langle(\Delta S_z)^2\rangle = 0$, as expected, since the system is in a well-defined eigenstate of S_z. In contrast, for the observable S_x, the dispersion is $\langle(\Delta S_x)^2\rangle = \frac{\hbar}{4}$, which is non-zero. This indicates that the system cannot be described by a well-defined eigenstate of S_x, and the value of this observable remains uncertain.

Postulate 3: The time evolution of the state vector $|\psi(t)\rangle_S$ is governed by the Schrödinger equation, where H is the operator associated with the total energy of the system (called the Hamiltonian):

$$i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle_S = H\left|\psi(t)\right\rangle_S, \tag{2.18}$$

where the subscript S in $\left|\psi(t)\right\rangle_S$ means the state is in the Schrödinger picture.

The Hamiltonian in quantum mechanics is defined similarly to the one in classical mechanics, given by the sum of the kinetic energy and potential energy

$$H = \frac{P^2}{2m} + V, \tag{2.19}$$

where P is the momentum operator and V is the potential energy. The solution of the Schrödinger equation gives the time-dependent state

$$\left|\psi(t)\right\rangle_S = U(t)\left|\psi(t_0)\right\rangle_S, \tag{2.20}$$

where the operator $U(t) = e^{\frac{-i}{\hbar}H(t-t_0)}$ is called the unitary time evolution operator. When the time dependence of the dynamical system is in the state, the state is in the Schrödinger picture.

A different way to describe the time evolution of a system is given by the Heisenberg picture, where, in this case, the observables evolve in time and the ket state is stationary. An observable A in the Heisenberg picture is given by

$$A_H(t) = U^\dagger(t)A_S U(t) = \sum_n a_n U^\dagger(t)\Lambda_{a_n}U(t) = \sum_n a_n \Lambda^H_{a_n}(t), \tag{2.21}$$

where the subscript S in $A_S = A_H(t_0)$ means the operator is in the Schrödinger representation and $\Lambda^H_{a_n}(t) = \left|a_n(t)\right\rangle\left\langle a_n(t)\right|$ are the projectors in the Heisenberg representation. This means that in the Schrödinger picture, the ket basis remain unchanged and the ket state evolves in time. In the Heisenberg picture, the ket state remains unchanged and the ket basis evolve in time in the opposite direction.

Taking the time derivative of the first two terms in equation (2.21)

$$\frac{d}{dt}A_H(t) = \frac{i}{\hbar}HU^\dagger(t)A_S U(t) - \frac{i}{\hbar}HU^\dagger(t)A_S U(t), \tag{2.22}$$

$$\frac{d}{dt}A_H(t) = \frac{i}{\hbar}[H, A_H(t)]. \tag{2.23}$$

This equation is called the Heisenberg equation of motion, which, similarly to the Schrödinger equation, governs the time evolution of an observable. An example of time evolution in a spin system will be given in the last section of this chapter.

2.2.1 Density Operator

Until now, the discussion has focused on the quantum mechanics of individual systems, described by their state $|\psi\rangle$. To describe an ensemble of systems, the density operator must be introduced. Consider an ensemble of systems with possible states $|\psi_n\rangle$, where p_n represents the probability of the system being in the state $|\psi_n\rangle$. The density operator ρ is then defined as

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i| = \sum_i p_i \rho_i, \tag{2.24}$$

which satisfy the following properties:

- Hermitian: $\rho = \rho^\dagger$.
- Unitary trace: $\mathrm{Tr}[\rho] = 1$.
- Positive semidefinite: $\langle\psi| \rho |\psi\rangle \geq 0$.

It is important to note that the probability p_i is associated with the lack of information about the system, analogous to the situation in classical physical systems. When the entire ensemble is in a single state $|\psi_i\rangle$ (i.e., $p_i = 1$), the density operator describes a pure state. Conversely, when the ensemble consists of subsystems in different configurations, the density operator represents a mixed state. As an example, consider a pure ensemble prepared in the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|z,+\rangle + |z,-\rangle)$. In this case, the density operator is given by

$$\rho_p = |\psi\rangle \langle\psi| = \frac{1}{2}(|z,+\rangle \langle z,+| + |z,+\rangle \langle z,-| + |z,-\rangle \langle z,+| + |z,-\rangle \langle z,-|). \tag{2.25}$$

Now, consider an ensemble in which half of the systems are in the state $|z,+\rangle$ and the other half are in the state $|z,-\rangle$. The density operator for this ensemble is given by

$$\rho_m = \frac{1}{2}(|z,+\rangle \langle z,+| + |z,-\rangle \langle z,-|), \tag{2.26}$$

which is clearly different from ρ_p. A useful criterion to determine whether a state is mixed is to compute the trace of its square. For any mixed state, the condition $\mathrm{Tr}[\rho^2] < 1$ holds, whereas for a pure state, $\mathrm{Tr}[\rho^2] = 1$ is satisfied. In the case of a maximally mixed state, $\rho_{mm} = \frac{\mathbb{1}}{d}$, where $d = \dim(\mathcal{H})$ and $\rho_{mm} \in \mathcal{H}$, the trace of its square is given by $\mathrm{Tr}[\rho_{mm}^2] = 1/d$.

The density operator also satisfies the postulates of quantum mechanics. The probability of observing the outcome a_n of a density operator ρ_i is

$$P_i(a_n) = \langle a_n| \rho_i |a_n\rangle, \tag{2.27}$$

so the probability $P(a_n)$ for the whole ensemble is the sum of the probabilities $P_i(a_n)$ weighted by p_i

$$P(a_n) = \sum_i p_i \, P_i(a_n) = \mathrm{Tr}[\Lambda_{a_n}\rho]. \tag{2.28}$$

The expectation value of an observable A can also be defined. By definition, it is given by

$$\langle A \rangle = \sum_n a_n P(a_n) = \mathrm{Tr}\left[\rho \sum_n a_n \Lambda_{a_n}\right] = \mathrm{Tr}[A\rho]. \tag{2.29}$$

The density operator right after a measurement is

$$\rho' = \frac{\Lambda_{a_n}\rho\Lambda_{a_n}}{\mathrm{Tr}[\Lambda_{a_n}\rho]}. \tag{2.30}$$

In the case where a measurement is performed but no information about the outcomes is available, the resulting state is described by a completely positive trace-preserving (CPTP) map:

$$\Phi_A(\rho) = \sum_n \Lambda_{a_n}\rho\Lambda_{a_n}. \tag{2.31}$$

The completely positive condition means that if this map (2.31) acts only on one part of the joint density operator, i.e.,

$$\Phi_A(\rho_{AB}) = \sum_n (\Lambda_{a_n} \otimes \mathbb{1}_B)\rho_{AB}(\Lambda_{a_n} \otimes \mathbb{1}_B), \tag{2.32}$$

then the resulting map must still be a density operator.

The density operator formalism is particularly useful for describing compound systems. For a bipartite system $\mathcal{H}_T = \mathcal{H}_A \otimes \mathcal{H}_B$, with respective bases $\{|a_n\rangle\}$ and $\{|b_m\rangle\}$, the density operator of the ensemble is denoted by ρ_{AB}. If the partial trace is taken with respect to the partition $\mathcal{H}_B$, then

$$\mathrm{Tr}_B(\rho_{AB}) = \sum_m \langle b_m| \rho_{AB} |b_m\rangle = \rho_A. \tag{2.33}$$

This result implies that for a bipartite system, the partial trace can be used to focus exclusively on the subsystem of interest.

The time evolution of density operators can now be defined. If the states $|\psi_i\rangle$ in ρ_i evolve in time as $|\psi_i(t)\rangle$, the time-dependent density operator is given by

$$\rho(t) = \sum_i p_i |\psi_i(t)\rangle \langle\psi_i(t)|. \tag{2.34}$$

From the fact that $|\psi_i(t)\rangle$ satisfies the Schrödinger equation, it follows that

$$\dot{\rho}(t) = \frac{i}{\hbar}\left[-H \sum_i p_i |\psi_i(t)\rangle \langle\psi_i(t)| + \sum_i p_i |\psi_i(t)\rangle \langle\psi_i(t)|\ H\right], \tag{2.35}$$

or

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho(t)], \tag{2.36}$$

which is similar to the Heisenberg equation in (2.23), but with the opposite sign. This is called the von Neumann equation, and similarly to the other equations of motion, it governs the time evolution of the density operator.

2.2.2 Information Theory

In information theory, a fundamental concept is the quantification of information gained after measuring an event. Consider an unbiased coin toss. After the coin is tossed, a measurement is performed to determine the outcome, thereby acquiring information about the state of the system.

An intuitive approach to quantifying information is to define it as the inverse of the probability: $I(x) = \frac{1}{p(x)}$, where $I(x)$ represents the information associated with the probability $p(x)$ of an event x [22]. For independent events, it is natural to expect that the joint information should be additive, i.e., $I(x,y) = I(x) + I(y)$. However, since the joint probability of independent events is $p(x,y) = p(x)p(y)$, the joint information would instead satisfy $I(x,y) = \frac{1}{p(x,y)} = \frac{1}{p(x)p(y)} \neq \frac{1}{p(x)} + \frac{1}{p(y)}$. To ensure the additivity of joint information, a logarithmic function can be introduced, allowing the information $I(x)$ to be redefined as

$$I(x) := \log_b \left(\frac{1}{p(x)} \right) = -\log_b p(x). \tag{2.37}$$

The base b of the logarithm determines the scale of information. When $b = 2$, the unit of information is referred to as a *bit*. In the case of an unbiased coin toss, for any possible outcome, the information gained is $I = -\log_2 \left(\frac{1}{1/2} \right) = 1$, indicating that one *bit* of information is acquired after the measurement.

For a random variable X with possible outcomes x_n, the mean averaged value for the random variable is

$$H(X) = \sum_p p(x_p) I(x_p) = -\sum_p p(x_p) \log_b p(x_p). \tag{2.38}$$

This quantity is known as the Shannon entropy [23]. It quantifies the amount of information gained from any observation made on the system. Conversely, the entropy also represents the uncertainty about the system prior to any measurement. For the case of an unbiased coin, $H(X) = 1$, indicating that the uncertainty is maximized before any measurement is performed. In contrast, for a biased coin that always results in heads, for example, $H(X) = 0$, reflecting the absence of uncertainty about the outcome, as only one result is possible. In the case of the biased coin, the limit $\lim_{x\to 0} x \log_2 x = 0$ has been used.

The Shannon entropy satisfy the following definitions:

- Binary entropy: The entropy of the two-outcome random variable X is given by

$$H_{bin}(X) := -p \log_b p - (1-p) \log_b (1-p), \tag{2.39}$$

where p and $(1-p)$ are the probabilities of the two possible outcomes.

- Conditional Entropy: after the knowing of Y, that is, in possession of the information $H(Y)$, the remaining uncertainty about the pair (X, Y) reduces to

$$H(X|Y) = H(X, Y) - H(Y), \tag{2.40}$$

where $H(X, Y) = \sum_{n,m} p(x_n, y_m) \log_b p(x_n, y_m)$ is the joint Shannon entropy.

In quantum mechanics, the uncertainty of a system can be quantified in a manner analogous to the Shannon entropy, known as the von Neumann entropy [24]. Consider a system described by the density operator ρ. The von Neumann entropy for this ensemble is defined as

$$S(\rho) := -\mathrm{Tr}[\rho \log_b \rho]. \tag{2.41}$$

Diagonalizing the operator ρ in an orthonormal basis, the von Neumann entropy becomes

$$S(\rho) = -\sum_n \lambda_n \log_b \lambda_n, \tag{2.42}$$

where λ_n are the eigenvalues of the density operator ρ. The von Neumann entropy must satisfy the following properties:

- Non-negative: $S(\rho) \geq 0$.
- Invariant under unitary transformation: $S(U\rho U^\dagger) = S(\rho)$.
- Maximum value: $S(\rho) = \log_b d$, for maximally mixed ensembles $\rho = \frac{\mathbb{1}}{d}$.
- Minimum Value: $S(\rho) = 0$, if and only if the ensemble is pure.
- Subadditivity for a bipartite ensemble: $S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B)$ with equality only when $\rho_{AB} = \rho_A \otimes \rho_B$.

Another important property is the non-decreasing nature of entropy under projective measurements. If a non-revealed measurement of a physical quantity A is performed, resulting in the state $\Phi_A(\rho)$, then

$$S(\Phi_A(\rho)) \geq S(\rho), \tag{2.43}$$

where $\Phi_A(\rho) = \sum_n \Lambda_{a_n} \rho \Lambda_{a_n}$.

Similarly to the classical case, the von Neumann entropy satisfy the following definitions:

- Quantum binary entropy: for an ensemble ρ with only two eigenvalues $\lambda_\pm$ that satisfy the relation $\lambda_+ = 1 - \lambda_-$, the entropy is given by

$$S(\rho) = -\lambda_+ \log_2 \lambda_+ - (1 - \lambda_+) \log_2 (1 - \lambda_+). \tag{2.44}$$

- Quantum conditional entropy: for a bipartite system ρ_{AB}, the conditional entropy of the subsystem ρ_A given ρ_B is

$$S(A|B) = S(\rho_{AB}) - S(\rho_B). \tag{2.45}$$

When there is no correlation between the subsystems $S(A|B) = S(\rho_A)$.

2.2.3 Probability Theory

The study of probability originated during the Renaissance era, motivated by the analysis of games of chance, such as calculating the likelihood of a specific outcome when rolling a die. In modern science, probabilistic methods are applied across diverse fields, including economics, chemistry, and physics. Given that quantum mechanics is fundamentally a probabilistic theory, a rigorous understanding of these concepts is essential for their application to quantum systems.

A rigorous foundation for probability theory was established in Andrey Kolmogorov's "Foundations of the Theory of Probability" [25], where the classical axioms of probability were first formally presented. This work systematized the mathematical framework that underlies both theoretical developments and practical applications in the field.

Before presenting these axioms, it is necessary to understand the concept of a measure space $(\Omega, \mathcal{F}, P)$. In this framework, Ω represents the sample space containing all possible outcomes of an experiment. For a fair coin toss, the sample space is $\Omega = \{H, T\}$, where H represents "heads" and T represents "tails". The σ-algebra $\mathcal{F}$ contains all measurable events, which for the coin toss example is $\mathcal{F} = \{\emptyset, \{H\}, \{T\}, \{H, T\}\}$. This mathematical structure provides the foundation for defining probability measures on discrete sample spaces.

The probability function P maps events to real numbers in the interval $[0, 1]$. There exist two predominant interpretations of probability in the literature. The frequentist interpretation defines probability as the limiting frequency of an event occurring in repeated experiments. In contrast, the Bayesian interpretation treats probability as a subjective degree of belief about an event [26]. These complementary perspectives both contribute to the rigorous foundation of probability theory and will be utilized in defining probability measures throughout this work.

Having established the definition of a measure space, we now present Kolmogorov's axioms of probability theory:

- **Non-Negativity**: For any event $E \in \mathcal{F}$,

$$P(E) \geq 0. \tag{2.46}$$

This implies that all probabilities must be non-negative. In the case of a fair coin, the probability measure satisfies $P(\{H\}) = P(\{T\}) = \frac{1}{2}$, $P(\varnothing) = 0$, and $P(\{H, T\}) = 1$.

- **Unit Measure**: The probability of the entire sample space Ω is 1,

$$P(\Omega) = 1. \tag{2.47}$$

The unit measure axiom states that the probability measure must account for all possible outcomes. In the case of a coin toss, this implies that exactly one of the two possible outcomes must occur with certainty.

- **Countable Additivity**: For a countable sequence of mutually exclusive (disjoint) events E_1, E_2, ...,

$$P\left(\bigcup_{i=1}^{\infty} E_i\right) = \sum_{i=1}^{\infty} P(E_i), \tag{2.48}$$

  where $E_i \cap E_j = \varnothing$ for $i \neq j$.

The countable additivity axiom states that the probability of a union of mutually exclusive events equals the sum of their individual probabilities. For a honest coin, the disjoint events $\{H\}$ and $\{T\}$ satisfy

$$P(\{H\} \cup \{T\}) = P(\{H\}) + P(\{T\}) = 1. \tag{2.49}$$

A direct consequence of this axiom is that for any event space consisting of mutually exclusive events, the union of all events equals the sample space:

$$P\left(\bigcup_{i=1}^{\infty} E_i\right) = P(\Omega). \tag{2.50}$$

Combining this with the unit measure axiom and countable additivity (2.48) yields

$$\sum_{i=1}^{\infty} P(E_i) = 1. \tag{2.51}$$

It is noteworthy that quantum mechanical probabilities also satisfy Kolmogorov's axioms. Recall that the positivity condition $\langle a_n | \rho | a_n \rangle \geq 0$ holds, and the probability of measuring outcome a_n is given by:

$$P(a_n) = \mathrm{Tr}[\Lambda_{a_n} \rho] = \langle a_n | \rho | a_n \rangle \geq 0. \tag{2.52}$$

It is straightforward to verify that the non-negativity axiom is satisfied. By employing the unit trace property, one can also demonstrate that quantum probabilities comply with the unit measure axiom. The probability associated with any observable outcome corresponds to the sum of all individual probabilities.

$$\sum_n P(a_n) = \sum_n \mathrm{Tr}[\Lambda_{a_n}\rho] = \mathrm{Tr}\left[\rho \sum_n \Lambda_{a_n}\right] = \mathrm{Tr}[\rho \mathbb{1}] = \mathrm{Tr}[\rho] = 1. \tag{2.53}$$

The linearity of the trace property is employed in this context. Finally, the countable additivity axiom can be demonstrated by invoking the linearity of the trace. Considering an orthonormal set of projectors representing disjoint outcomes, the probability of disjoint events is expressed as

$$P\left(\bigcup_{i=1}^{\infty} E_i\right) = P\left(\bigoplus_{n=1}^{\infty} \Lambda_{a_n}\right), \tag{2.54}$$

where $\bigoplus_{n=1} \Lambda_{a_n}$ represents the sum of the subsets of the projectors. Expanding (2.54)

$$P\left(\bigoplus_{n=1} \Lambda_{a_n}\right) = \mathrm{Tr}\left[\rho \sum_n \Lambda_{a_n}\right] = \sum_n \mathrm{Tr}[\Lambda_{a_n}\rho] = \sum_n P(a_n), \tag{2.55}$$

thus showing that the three Kolmogorov axioms of the probability theory are satisfied by the quantum theory.

The probability functions presented thus far refer to single events involving a single measurement. However, there are situations in which it is necessary to compute the probability of two or more events. To address this, three important probability functions will be introduced in this context: the joint probability, the marginal probability, and the conditional probability (for further details, see [27]). Before proceeding, it is necessary to define the concept of a random variable.

A random variable is a mathematical construct used to quantify random phenomena within the framework of probability theory. Denoting a random variable by the capital letter X, its domain corresponds to the sample space of the system under consideration, $\Omega = \{x\}$, and its range associates each outcome with a numerical value. By convention, outcomes are denoted by lowercase letters, so the probability of observing a specific outcome x is represented as $P(X = x)$.

When two events occur and it is necessary to describe the probability of both events happening together, the joint probability is used. For two systems with different random variables $X = x$ and $Y = y$, their joint probability is written as $P(X = x, Y = y)$. In the case where these random variables are independent of one another, the joint probability is given by the product of the individual probabilities of each random variable.

$$P(X = x, Y = y) = P(X = x)P(Y = y). \tag{2.56}$$

As an example, for two honest coins, the probability of measuring heads in both of them is

$$P(X = 1, Y = 1) = P(X = 1)P(Y = 1) = \frac{1}{2}\frac{1}{2} = \frac{1}{4}. \tag{2.57}$$

Similarly to the individual probabilities, the joint probabilities must be positive and sum up to one

$$\sum_{x,y} P(X = x, Y = y) = 1, \tag{2.58}$$

where the sum is taken over all possible events of X and Y. Using the joint probability, it is also possible to describe the individual behaviour of one of the random variables through the marginal probability. For independent random variables X and Y, the individual probability of $X = x$ is

$$P(X = x) = \sum_{y} P(X = x, Y = y). \tag{2.59}$$

Given that the probability function $P(Y = y)$ satisfy the Kolmogorov axioms, then

$$P(X = x) = P(X = x) \sum_{y} P(Y = y) = P(X = x), \tag{2.60}$$

where $\sum_y P(Y = y) = 1$. It is important to emphasize that the marginal probability can only be used for random variables that are independent of one another. In cases where the random variables are correlated, the probabilities of the events must be defined using conditional probabilities.

Imagine a professor who eats lunch at a restaurant near the physics department. The menu of the day is either chicken or steak, each with a 50% probability. When the menu is chicken, there's a 70% chance he eats cake for dessert and a 30% chance he eats fruit. When the menu is steak, there's a 20% chance he eats cake and an 80% chance he eats fruit. In this case, the choice of dessert is probabilistically dependent on the menu: knowing whether the menu is chicken or steak changes the probability of the dessert. Thus, the menu and the dessert are correlated events.

For two dependent random variables X and Y, the conditional probability of the event $X = x$ given that $Y = y$ was measured is

$$lP(X = x|Y = y) = \frac{P(X = x, Y = y)}{P(y = y)}. \tag{2.61}$$

In the expression (2.61), the joint probability is not factorizable, since the events are correlated. Isolating the joint probability and rewriting the conditional probability for the event $Y = y$ given that $X = x$ was measured, one can deduce the Bayes rule

$$P(Y = y|X = x) = \frac{P(X = x|Y = y)P(Y = y)}{P(X = x)}. \tag{2.62}$$

The Bayes rule can be really useful when one wants to determine a conditional probability, but only knows in the reverse order.

2.3 Qubit Formalism

The spin $1/2$ system, or simply a qubit, is extremely useful for discussing quantum mechanics in all subjects, as we have shown so far. Because of this, we need to make a more profound discussion on this subject. The spin operators are $S_n = \frac{\hbar}{2}\sigma_n$, where n is a given direction. The Pauli matrices σ_n in three orthogonal directions are written as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.63}$$

with the respective eigenstates

$$|x,+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |x,-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{2.64}$$

$$|y,+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |y,-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}, \tag{2.65}$$

$$|z,+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |z,-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.66}$$

The kets $|n,+\rangle$ are the eigenstates associated with the positive eigenvalues $(+1)$ and the $|n,-\rangle$ are the ones associated with the negative eigenvalues (-1). The Pauli matrices are involutory ($\sigma_n^2 = \mathbb{1}$), traceless ($\mathrm{Tr}[\sigma_n] = 0$), Hermitian ($\sigma_n = \sigma_i^\dagger$) and satisfy the following commutation relation

$$[\sigma_i, \sigma_j] = 2i\, \epsilon_{ijk}\, \sigma_k, \tag{2.67}$$

where ϵ_{ijk} is the Levi-Civita symbol. There are cases where observations are not made along one of the three orthogonal directions x, y, or z, but rather along a linear combination of them. For such cases, the projection of a given unit vector $\hat{r}$ onto the Pauli vector $\vec{\sigma}$ is used, resulting in the following operator

$$\sigma_{\hat{r}} = (r_x\, \hat{x} + r_y\, \hat{y} + r_z\, \hat{z}) \cdot (\sigma_x\, \hat{x} + \sigma_y\, \hat{y} + \sigma_z\, \hat{z}) = \hat{r} \cdot \vec{\sigma}, \tag{2.68}$$

or in the matrix representation

$$\sigma_{\hat{r}} = \begin{pmatrix} r_z & r_x - ir_y \\ r_x + ir_y & -r_z \end{pmatrix}. \tag{2.69}$$

As demonstrated, the Pauli vector provides a mapping mechanism from a vector basis $(\hat{r})$ to a Pauli matrix basis. This mapping preserves all the properties of the Pauli matrices.

There are two key identities involving Pauli vectors that are relevant to this work. The first is the product of two Pauli vectors in different directions. Consider two distinct unit vectors $\hat{a} = (a_1, a_2, a_3)$ and $\hat{b} = (b_1, b_2, b_3)$. The product of the Pauli matrices in these directions is given by

$$(\hat{a} \cdot \vec{\sigma})(\hat{b} \cdot \vec{\sigma}) = \begin{bmatrix} a_1b_1 + a_2b_2 + a_3a_3 - i(a_2b_1 - a_1b_2) & a_3b_1 - a_1b_3 - i(a_3b_2 - a_2b_3) \\ -a_3b_1 + a_1b_3 - i(a_3b_2 - a_2b_3) & a_1b_1 + a_2b_2 + a_3a_3 + i(a_2b_1 - a_1b_2) \end{bmatrix}. \tag{2.70}$$

The first three elements in the diagonal of this matrix are simply the dot product of the vectors $\hat{a} \cdot \hat{b}$. From this, this matrix can be rewritten as

$$(\hat{a}\cdot\vec{\sigma})(\hat{b}\cdot\vec{\sigma}) = (\hat{a}\cdot\hat{b})\mathbb{1}+i \begin{bmatrix} -(a_2b_1 - a_1b_2) & -i(a_3b_1 - a_1b_3) - (a_3b_2 - a_2b_3) \\ -i(-a_3b_1 + a_1b_3) - (a_3b_2 - a_2b_3) & (a_2b_1 - a_1b_2) \end{bmatrix}. \tag{2.71}$$

It is easy to see that the elements in the second matrix are the components of the vector $\hat{a} \times \hat{b}$ and the similarity to the matrix of (2.69) becomes much clear. From this, we will have the final form of the product of two Pauli matrices in different directions

$$(\hat{a} \cdot \vec{\sigma})(\hat{b} \cdot \vec{\sigma}) = (\hat{a} \cdot \hat{b})\mathbb{1} + i(\hat{a} \times \hat{b}) \cdot \vec{\sigma}. \tag{2.72}$$

An interesting application of the equation (2.72) is in the commutator of spin operators in different directions. For two unity vectors $\hat{a}$ and $\hat{b}$, the spin operators $\hat{a} \cdot \vec{\sigma}$ and $\hat{b} \cdot \vec{\sigma}$ have the following commutator

$$\begin{aligned} [\hat{a} \cdot \vec{\sigma}, \hat{b} \cdot \vec{\sigma}] &= (\hat{a} \cdot \hat{b})\mathbb{1} + i(\hat{a} \times \hat{b}) \cdot \vec{\sigma} - (\hat{a} \cdot \hat{b})\mathbb{1} - i(\hat{b} \times \hat{a}) \cdot \vec{\sigma} \\ [\hat{a} \cdot \vec{\sigma}, \hat{b} \cdot \vec{\sigma}] &= 2i(\hat{a} \times \hat{b}) \cdot \vec{\sigma}. \end{aligned} \tag{2.73}$$

If the vectors $\hat{a}$ and $\hat{b}$ are orthogonal to each other, then the relation in (2.73) returns to (2.67). A relation that will be used is the norm of the commutation relation of the Pauli vectors. The squared norm of an operator A is given by

$$||A||^2 = \mathrm{Tr}[A^\dagger A]. \tag{2.74}$$

Having that the product of the commutator (2.73) and its dagger is

$$[\hat{a} \cdot \vec{\sigma}, \hat{b} \cdot \vec{\sigma}]^\dagger [\hat{a} \cdot \vec{\sigma}, \hat{b} \cdot \vec{\sigma}] = [4 - 4(\hat{a} \cdot \hat{b})^2]\mathbb{1}_2, \tag{2.75}$$

where we used the identity $(\vec{a} \times \vec{b}) \cdot (\vec{c} \times \vec{d}) = (\vec{c} \cdot \vec{a})(\vec{b} \cdot \vec{d}) - (\vec{b} \cdot \vec{c})(\vec{a} \cdot \vec{d})$. If $A = [\hat{a} \cdot \vec{\sigma}, \hat{b} \cdot \vec{\sigma}]$, the norm of the commutator becomes

$$||[\hat{a} \cdot \vec{\sigma}, \hat{b} \cdot \vec{\sigma}]||^2 = 8 - 8(\hat{a} \cdot \hat{b})^2. \tag{2.76}$$

The second important identity is the complex exponential of the Pauli matrix. Suppose a Pauli matrix given by $\vec{\theta} \cdot \vec{\sigma}$, where $\vec{\theta} = \theta\hat{n}$. Then, the Taylor series for this exponential function will be

$$e^{i\theta(\hat{n}\cdot\vec{\sigma})} = \sum_{k=0}^{\infty} \frac{i^k[\theta(\hat{n} \cdot \vec{\sigma})^k]}{k!} = \sum_{p=0}^{\infty} \frac{(-1)^p[\theta(\hat{n} \cdot \vec{\sigma})^{2p}]}{(2p)!} + \sum_{q=0}^{\infty} \frac{(-1)^q[\theta(\hat{n} \cdot \vec{\sigma})^{2q+1}]}{(2q+1)!}. \tag{2.77}$$

Remembering the Taylor series expansion for the cosine and sine functions and invoking the involutionary property of the Pauli matrices

$$e^{i\theta(\hat{n}\cdot\vec{\sigma})} = \mathbb{1}\cos\theta + i(\hat{n}\cdot\vec{\sigma})\sin\theta. \tag{2.78}$$

Now, let us propose an example of a dynamical system for the qubit. Consider a qubit interacting with a homogeneous magnetic field $\vec{B} = B\hat{h}$. The Hamiltonian for this system is given by $H = -\vec{S}\cdot\vec{B} = \frac{\hbar}{2}\omega(\hat{h}\cdot\vec{\sigma})$, where $\omega = -\frac{eB}{m_e}$ is the Larmor frequency. The time evolution of the spin operator in the $\hat{n}$ direction, S_n, is described by

$$S_{\hat{n}}(t) = U^{\dagger}(t) S_n U(t), \tag{2.79}$$

$$S_{\hat{n}}(\tau) = \frac{\hbar}{2} e^{\frac{i\hat{h}\cdot\sigma\tau}{2}} (\hat{n}\cdot\vec{\sigma}) e^{\frac{-i\hat{h}\cdot\sigma\tau}{2}}, \tag{2.80}$$

where we introduced the normalized time $\tau = \omega t$. With the identity (2.78), we have

$$S_{\hat{n}}(\tau) = \frac{\hbar}{2}\left[\mathbb{1}\cos\left(\frac{\tau}{2}\right) + i(\hat{h}\cdot\vec{\sigma})\sin\left(\frac{\tau}{2}\right)\right](\hat{n}\cdot\vec{\sigma})\left[\mathbb{1}\cos\left(\frac{\tau}{2}\right) - i(\hat{h}\cdot\vec{\sigma})\sin\left(\frac{\tau}{2}\right)\right], \tag{2.81}$$

$$\begin{aligned} S_{\hat{n}}(\tau) = \frac{\hbar}{2}\Big[&\cos^2\left(\frac{\tau}{2}\right)(\hat{n}\cdot\vec{\sigma}) - i\sin\left(\frac{\tau}{2}\right)\cos\left(\frac{\tau}{2}\right)(\hat{n}\cdot\vec{\sigma})(\hat{h}\cdot\vec{\sigma}) \\ &+ i\sin\left(\frac{\tau}{2}\right)(\hat{h}\cdot\vec{\sigma})(\hat{n}\cdot\vec{\sigma}) + \sin^2\left(\frac{\tau}{2}\right)(\hat{h}\cdot\vec{\sigma})(\hat{n}\cdot\vec{\sigma})(\hat{h}\cdot\vec{\sigma})\Big]. \end{aligned} \tag{2.82}$$

With (2.72), we have the final form of the spin operator in a general direction in the Heisenberg picture:

$$S_{\hat{n}}(\tau) = \frac{\hbar}{2}\{\cos\tau\ \hat{n} + \sin\tau(\hat{n}\times\hat{h}) + [1-\cos\tau](\hat{h}\cdot\hat{n})\hat{h}\}\cdot\vec{\sigma}, \tag{2.83}$$

$$S_{\hat{n}}(\tau) = \frac{\hbar}{2}\hat{m}(\tau)\cdot\vec{\sigma}, \tag{2.84}$$

where

$$\hat{m}(\tau) = \{\cos\tau\ \hat{n} + \sin\tau(\hat{n}\times\hat{h}) + [1-\cos\tau](\hat{h}\cdot\hat{n})\hat{h}\}. \tag{2.85}$$

In the case where $\hat{n} \parallel \hat{h}$, the observable becomes $S_n(\tau) = \hat{n}\cdot\vec{\sigma}$, which is expected since the precession process occur only in the plane perpendicular from $\hat{h}$ and the operator will be stationary. If $\hat{n}\perp\hat{h}$, then $S_n(\tau) = \frac{\hbar}{2}[\cos\tau\ \hat{n} + \sin\tau\ \hat{v}]\cdot\vec{\sigma}$ where $\hat{v}\perp\hat{h}$ and $\hat{v}\perp\hat{n}$. If $\hat{h} = \hat{z}$ and $\hat{n} = \hat{x}$, then $\hat{v} = \hat{y}$ and the observable becomes $S_x = \frac{\hbar}{2}\cos\tau\ \sigma_x$, which is a well known result for the spin precessing dynamics.

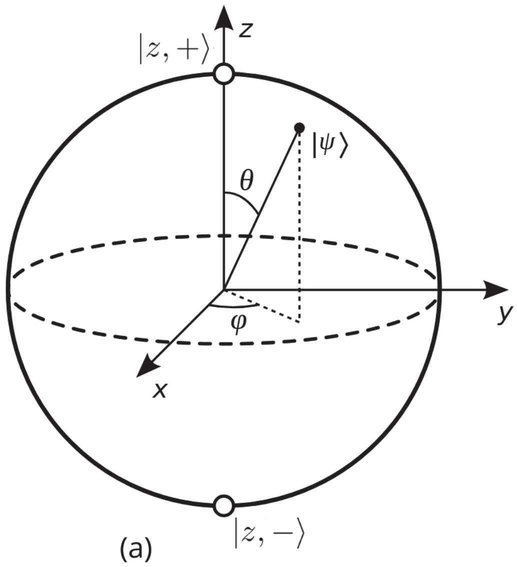
2.3.1 Bloch Representation

Since qubits are two-level systems, a general state for a given direction $\hat{r}$ can be written as the superposition of the two possible states $|\psi\rangle = \frac{1}{\sqrt{2}}(|\hat{r},+\rangle + |\hat{r},-\rangle)$. But we can also describe the system for every possible direction using one state by the

Bloch representation, in which the possible states are points in the surface of a sphere centered at the origin (Figure 3 (a)). In this representation, the state $|\psi\rangle$ becomes

$$|\psi\rangle = \cos\left(\theta/2\right)|z,+\rangle + e^{i\phi}\sin\left(\theta/2\right)|z,+\rangle\,, \tag{2.86}$$

where the angles $\theta \in [0,\pi]$ and $\phi \in [0,2\pi]$ are the components of a vector in spherical coordinates. The possible choices of the angles that give the eigenstates of the Pauli matrices are shown in the Figure 3 (b).



(a)

θ	ϕ	$\|\psi\rangle$
0	0	$\|z,+\rangle$
π	0	$\|z,-\rangle$
$\pi/2$	0	$\|x,+\rangle$
$\pi/2$	π	$\|x,-\rangle$
$\pi/2$	$\pi/2$	$\|y,+\rangle$
$\pi/2$	$3\pi/2$	$\|y,-\rangle$

(b)

Figure 3 – (a) Diagram of the Bloch sphere. Font: Wikipedia[1]. (b) Table of the possible values of θ and ϕ with theirs respective state.

The pure density operator associated with the state in (2.86) is

$$\begin{aligned}
\rho_{\hat{r}} &= |\psi\rangle\langle\psi| \qquad (2.87)\\
&= \begin{pmatrix} \cos^2\left(\theta/2\right) & \sin\left(\theta/2\right)\cos\left(\theta/2\right)e^{-i\phi} \\ \sin\left(\theta/2\right)\cos\left(\theta/2\right)e^{i\phi} & \sin^2\left(\theta/2\right) \end{pmatrix}\\
&= \begin{pmatrix} \frac{1+\cos\theta}{2} & \frac{e^{-i\phi}\sin\theta}{2} \\ \frac{e^{i\phi}\sin\theta}{2} & \frac{1+\sin\theta}{2} \end{pmatrix}\\
&= \frac{1}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin\theta\cos\phi\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin\theta\sin\phi\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos\theta\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\right]\\
&= \frac{\mathbb{1} + \hat{r}\cdot\vec{\sigma}}{2}, \qquad (2.88)
\end{aligned}$$

with the vector unity $\hat{r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. The purity of the state can be easily demonstrated since

$$\rho_{\hat{r}}^2 = \frac{\mathbb{1} + 2\hat{r}\cdot\vec{\sigma} + (\hat{r}\cdot\vec{\sigma})^2}{4} = \frac{\mathbb{1} + \hat{r}\cdot\vec{\sigma}}{2}, \tag{2.89}$$

[1] Available at: https://en.wikipedia.org/wiki/Bloch_sphere. Accessed: February 10th, 2025.

and with the traceless property, $\mathrm{Tr}[\rho_{\hat{r}}^2] = 1$, as expected. In the case where we want to define a mixed state in the Bloch sphere, it is possible to change the unit vector $\hat{r}$ to the vector $\vec{r} = (\sin\theta\cos\phi\, r, \sin\theta\sin\phi\, r, \cos\theta\, r)$, giving the state

$$\rho_{\vec{r}} = \frac{\mathbb{1} + \vec{r}\cdot\vec{\sigma}}{2}, \tag{2.90}$$

with the following eigenvalues

$$\lambda_{\pm} = \frac{1}{2}(1 \pm \|\vec{r}\|). \tag{2.91}$$

The square of the state $\rho_{\vec{r}}$ is

$$\rho_{\vec{r}}^2 = \frac{\mathbb{1} + 2\vec{r}\cdot\vec{\sigma} + (\vec{r}\cdot\vec{\sigma})^2}{4} = \frac{\mathbb{1} + 2\vec{r}\cdot\vec{\sigma} + \mathbb{1}\|\vec{r}\|^2}{4}, \tag{2.92}$$

with trace $\mathrm{Tr}[\rho_{\vec{r}}^2] = \frac{1}{2}(1 + r^2)$, where $\|\vec{r}\| = r$ and $0 \leq r \leq 1$, so $\rho_{\vec{r}}$ is positive-semidefinite. The trace $\mathrm{Tr}[\rho_{\vec{r}}^2]$ indicates that in the Bloch representation, the pure states are located on the outer shell of the sphere, while the mixed ones are in the inner volume.

In cases where no prior information about the system is available, multiple observations of the physical quantities characterizing the system can be performed to reconstruct the density operator. This process is known as state tomography [28]. For a spin system, this reconstruction can be achieved by measuring the components of the spin vector, such that

$$\langle S_x \rangle = \mathrm{Tr}[S_x \rho_r] = \frac{\hbar}{2} r_x \tag{2.93a}$$

$$\langle S_y \rangle = \mathrm{Tr}[S_y \rho_r] = \frac{\hbar}{2} r_y \tag{2.93b}$$

$$\langle S_z \rangle = \mathrm{Tr}[S_z \rho_r] = \frac{\hbar}{2} r_z, \tag{2.93c}$$

where the terms r_x, r_y, and r_z are the components of the vector $\vec{r}$ from the state $\rho_{\vec{r}}$. After numerous observations, the components of the vector will become better defined, and we will be able to reconstruct the state. This discussion will be explored in future chapters.

CHAPTER 3

Time as Which Way Information

3.1 Time-Energy Uncertainty Principle

Time can be a difficult subject to define in physics. In [29, 30], Paul Busch says that in physics there exist three possible kinds of time : external time, intrinsic time, and observable time.

The external time is the period which intermediates changes in some dynamical system measured by external equipment that does not have any interaction with the system itself. External time is sharply defined for all experiments and does not have any uncertainty interpretation. This kind of time is the one seen in classical physics.

The intrinsic time is associated with the evolution of some dynamical variable, which marks the passage of time by the change of its states, like the angle of a pendulum or the position a free particle. An interesting application of this kind of time is in the Mandelstam-Tamm relation [31, 32] (the observable time will be discussed in the next section).

Consider a classical dynamical variable $\mathrm{C} = \mathrm{C}(t)$, which serves as a measure of time, analogous to the pointers of a clock. If $\Delta\mathrm{C}$ represents the uncertainty in C over a time interval Δt, then

$$\Delta\mathrm{C} = \left|\frac{d\mathrm{C}}{dt}\right|\Delta t. \tag{3.1}$$

To apply this identity to the quantum case, the dynamical variable $\mathrm{C}(t)$ is promoted to an operator, $\mathrm{C}(t) \to C(t)$. It is important to note that the time dependence in $C(t)$ arises from the time evolution generated by the Hamiltonian H, rather than any implicit time dependence. By the correspondence principle, the classical variable is replaced with the expectation value of the corresponding observable, such that

$$\Delta C = \left|\frac{d\langle C\rangle}{dt}\right|\Delta t(C). \tag{3.2}$$

The quantity ΔC is the dispersion of the observable C and $\Delta t(C)$ a period of time. An interpretation for this equation is that, with an increase in the time scale over which an observation is made, the uncertainty of the physical observable will also increase. Using the generalized Ehrenfest theorem [33]

$$i\hbar\frac{d\langle C\rangle}{dt} = \langle[C, H]\rangle. \tag{3.3}$$

Substituting (3.3) into (3.2)

$$\Delta C = \frac{1}{\hbar}|\langle[C, H]\rangle|\Delta t(C). \tag{3.4}$$

Applying this result to (2.17) for $A = C$ and $B = H$, the Mandelstam-Tamm uncertainty relation is obtained:

$$\Delta E\Delta t(C) \geq \frac{\hbar}{2}. \tag{3.5}$$

where $\Delta E = \langle(\Delta H)^2\rangle$. It is important to rephrase that, in this case, differently from the uncertainty relation proposed in (2.17), the value of $\Delta t(C)$ does not represent the dispersion of the observable, since time is not treated as a physical quantity. In fact, Mandelstam-Tamm say that $\Delta t(C)$ *represents the amount of time it takes the expectation value of any quantum observable* C *to change by one dispersion* ΔC.

3.2 Observable Time

The time-energy uncertainty principle was initially proposed by Heisenberg [34], where he defined that there was an operator for the observable time and another for the energy, which is called the Hamiltonian. In his work, he did not take into account the consequences of such a definition. Years later, Pauli argued that it is not possible for a self-adjoint time operator to exist in conjunction with a Hamiltonian that has a lower bound [13]. This became known as the Pauli objection, which is formally defined as:

- Pauli's objection: Consider a physical system whose Hamiltonian H is bounded from below. Then, it is not possible to construct a self-adjoint operator T such that

$$[T, H] = i\hbar\mathbb{1}. \tag{3.6}$$

The hypothesis that the Hamiltonian is bounded from below means that there exists a energy eigenstate $|E_0\rangle$ with energy E_0 such that $E \geq E_0$ where E represents all the possible energy levels allowed in the system. This hypothesis comes from what is seen in nature, such as the quantized electromagnetic field, which do have a ground state.

Now, let us prove Pauli's objection by contradiction. Suppose there exists a self-adjoint operator T and a unitary operator $U_\lambda = e^{-i\lambda T}$, where $\lambda \in \mathbb{R}$. The unitarity of U_λ follows directly from the assumption that T is self-adjoint, i.e., $T = T^\dagger$. The expansion of the commutator of the unitary operator U_λ and the Hamiltonian H yields [35]:

$$[U_\lambda, H] = \sum_k \frac{(-i\lambda)^k}{k!}[T^k, H] = -\lambda U_\lambda. \tag{3.7}$$

Let $|E\rangle$ be an eigenstate of H. It is a direct consequence of the commutation relation (3.7) that

$$HU_\lambda |E\rangle = (U_\lambda H - [U_\lambda, H]) |E\rangle = (E + \lambda)U_\lambda |E\rangle . \tag{3.8}$$

This means that $U_\lambda |E\rangle$ is an eigenstate of H, which implies that the spectrum of eigenvalues of H spans the entire real line. Consequently, the Hamiltonian does not have a lower bound, thereby completing the proof.

In next two sections, we will show two approach of time as an observable. The first is the Aharonov-Bohm time observable [14], which satisfy the Pauli objection. The second is in the Page-Wootters mechanism [15], which bypasses the objection.

3.2.1 Aharonov-Bohm Time Operator

Let us consider a free particle with the Hamiltonian given by

$$\mathrm{H} = \frac{\mathrm{p}^2}{2m}, \tag{3.9}$$

where p is the momentum of the particle and m its mass. The interval of time it takes to the particle positioned at $\mathrm{x}(t_0 = 0) = \mathrm{x}_0$ and velocity $\mathrm{v} = \frac{\mathrm{p}}{m}$ to travel to $\mathrm{x} = 0$ is

$$t - t_0 = \frac{\mathrm{x} - \mathrm{x}_0}{\mathrm{v}} \to t = -\frac{\mathrm{x}_0 m}{\mathrm{p}} = -m\mathrm{x}_0\mathrm{p}^{-1}. \tag{3.10}$$

This is the time of arrival at the origin. If the time is negative, it means that the particle already passed at the origin in the instant $t = 0$. Using the symmetrization rule in equation (3.10)

$$T = -\frac{m}{2}(P^{-1}X + XP^{-1}), \tag{3.11}$$

where X and P are the position and momentum operator, respectively. This operator is called the Aharonov-Bohm time operator, since it was first proposed by them in the paper [14]. This operator is Hermitian

$$T^\dagger = -\frac{m}{2}[(P^{-1}X)^\dagger + (XP^{-1})^\dagger] = -\frac{m}{2}[X^\dagger(P^\dagger)^{-1} + (P^\dagger)^{-1}X^\dagger] = T, \tag{3.12}$$

and also satisfy the relation in (3.6) for the Hamiltonian of the free particle

$$\begin{aligned}
[H,T] &= -\frac{1}{4}([P^2, XP^{-1}] + [P^2, P^{-1}X]) \\
&= -\frac{1}{4}(P^2XP^{-1} - XP^{-1}P^2 + P^2P^{-1}X - P^{-1}XPP) \\
&= -\frac{1}{4}(P([P,X] + XP)P^{-1} - XP + PX - P^{-1}X([X,P] + PX)P) \\
&= -\frac{1}{4}(P(-i\hbar\mathbb{1} + XP)P^{-1} - XP + PX - P^{-1}(i\hbar\mathbb{1} + PX)P) \\
&= -\frac{1}{4}(-i\hbar\mathbb{1} + PX - XP + PX - i\hbar\mathbb{1} - XP) \\
&= -\frac{1}{4}(2[X,P] + 2i\hbar\mathbb{1}) \\
&= i\hbar\mathbb{1},
\end{aligned} \tag{3.13}$$

where the canonical commutation relation $[X,P] = i\hbar\mathbb{1}$ has been used. The spectrum of eigenvalues of the Hamiltonian is

$$H\,|E\rangle = E\,|E\rangle \to E = \frac{p^2}{2m}. \tag{3.14}$$

Having that $p \in \mathbb{R}$, then $E \geq 0$ and the Hamiltonian of the free particle has a lower bound. Thus, by the Pauli objection the time operator T must not be self-adjoint.

The distinction between self-adjoint operators and Hermitian (or symmetric) operators is only relevant for infinite-dimensional Hilbert spaces, which is the case here. An operator is said to be Hermitian if $D(T) \subset D(T^\dagger)$ and $T\,|\phi\rangle = T^\dagger\,|\phi\rangle$, where $D(T)$ represents the eigensubspace of the operator $T : \mathcal{H} \to \mathcal{H}$ and $\{|\phi\rangle\} \in D(T)$. An operator is said to be self-adjoint if it is Hermitian and if $D(T) = D(T^\dagger)$ [36]. So, all self-adjoint operators are Hermitian, but not all Hermitian operators are self-adjoint. A direct consequence of the time operators not been self-adjoint is that its eigenstates will not be orthogonal.

The objective now is to construct a POVM (positive operator-valued measure) in $\mathbb{R}$ for the time operator T, enabling the computation of probabilities for time measurements. To achieve this, it is necessary to define the eigenstates $|t\rangle$, such that

$$T\,|t\rangle = t\,|t\rangle\,, \tag{3.15}$$

where $t \in \mathrm{R}$. Rewriting (3.11) in the momentum representation and defining that $\phi_t(p) = \langle p|t\rangle$ is the wave function of the state $|t\rangle$ in the momentum representation

$$\begin{aligned}
\langle p|\,T\,|t\rangle &= t\phi_t(p) \\
&= -\frac{im}{2}\,\langle p|\left(\frac{d}{dp}\left[\frac{1}{p}\right] + \frac{1}{p}\frac{d}{dp}\right)|t\rangle \\
&= -\frac{im}{2}\left(\frac{d}{dp}\left[\frac{\phi_t(p)}{p}\right] + \frac{1}{p}\frac{d\phi_t(p)}{dp}\right) \\
&= \frac{im}{2}\left(\frac{\phi_t(p)}{p^2} - \frac{2}{p}\frac{d\phi_t(p)}{dp}\right),
\end{aligned} \tag{3.16}$$

which gives the following differential equation:

$$\frac{d\phi_t(p)}{dp} = \left[\frac{1}{2p} + \frac{ipt}{m}\right]\phi_t(p). \tag{3.17}$$

Due to the divergence at $p = 0$, this differential equation admits two families of eigenfunctions: one for $p > 0$ and another for $p < 0$. Introducing a constant $\alpha = \pm 1$, where $\alpha = 1$ corresponds to the eigenfunction with $p > 0$ and $\alpha = -1$ corresponds to the eigenfunction with $p < 0$, the solutions to (3.17) are given by

$$\phi_{t,\alpha}(p) = \frac{1}{\sqrt{2\pi m}}\Theta(\alpha p)\sqrt{|p|}e^{\frac{ip^2 t}{2m}}. \tag{3.18}$$

where $\Theta(\alpha p)$ is the Heaviside step function:

$$\Theta(\alpha p) = \begin{cases} 1, & if \;\; \alpha p \geq 0 \\ 0, & if \;\; \alpha p < 0. \end{cases} \tag{3.19}$$

It is important to note that the eigenfunctions $\phi_{t,\alpha}(p)$ do not belong to the Hilbert space of square-integrable functions, as they are not normalizable. However, similar to the case of plane waves (wave functions of the position eigenstates in the momentum representation), the state $|t, \alpha\rangle$ can be associated with the wave functions $\phi_{t,\alpha}(p)$, such that

$$\langle p|t, \alpha\rangle = \phi_{t,\alpha}(p) = \frac{1}{\sqrt{2\pi m}}\Theta(\alpha p)\sqrt{|p|}e^{\frac{ip^2 t}{2m}}. \tag{3.20}$$

But this analogy has a problem since the eigenstates of the time operator are not orthogonal, in the sense they do not satisfy relations like

$$\langle x|x'\rangle = \delta(x - x') \;\; and \;\; \langle p|p'\rangle = \delta(p - p'). \tag{3.21}$$

For the case where $\alpha \neq \alpha'$, the inner product of $|t, \alpha\rangle$ and $|t', \alpha'\rangle$ is

$$\langle t, \alpha|t', \alpha'\rangle = \int dp \, \langle t, \alpha|p\rangle \, \langle p|t', \alpha'\rangle \tag{3.22}$$

$$\langle t, \alpha|t', \alpha'\rangle = \frac{1}{2\pi m}\int dp\Theta(p)\Theta(-p)|p|e^{\frac{ip^2(t'-t)}{2m}} = 0. \tag{3.23}$$

For the case where $\alpha = \alpha' = 1$

$$\langle t, \alpha|t', \alpha\rangle = \frac{1}{2\pi m}\int dp \; \Theta(p)|p|e^{\frac{ip^2(t'-t)}{2m}} = \frac{1}{2\pi m}\int_0^\infty dp \; pe^{\frac{ip^2(t'-t)}{2m}}. \tag{3.24}$$

The last term in (3.24) corresponds to the Fourier transform of the Heaviside step function. Thus, we obtain

$$\langle t, \alpha|t', \alpha\rangle = \frac{1}{2}\delta(t' - t) + \frac{i}{2\pi(t' - t)}. \tag{3.25}$$

Therefore, the eigenstates of the time operator do not form a orthogonal base in the Hilbert space, which is expected, since we already stated that the time operator T is not self-adjoint. But the operator $|t,\alpha\rangle\langle t,\alpha|$ satisfy a completeness relation. Given that

$$\sum_{\alpha=\pm1}\int dt\,\langle p'|t,\alpha\rangle\langle t,\alpha|p\rangle=\frac{1}{2\pi m}\int dt\,\sqrt{|p|}\sqrt{|p'|}\Theta(\alpha p)\Theta(\alpha p')e^{\frac{it(p^2-(p')^2)}{2m}}. \tag{3.26}$$

Having the Dirac's delta function integral representation

$$\delta(x-x')=\frac{1}{2\pi}\int dte^{it(x-x')}, \tag{3.27}$$

we get

$$\frac{1}{2\pi m}\int dte^{\frac{it(p^2-(p')^2)}{2m}}=\frac{1}{m}\delta\left(\frac{p^2}{2m}-\frac{(p')^2}{2m}\right). \tag{3.28}$$

Using another Dirac's delta property, which says that for a given function $g(x)$ such that $g(x_i)=0$ for $i=1,...,n$ [37]

$$\delta(g(x))=\sum_{i=1}^{n}\frac{\delta(x-x_i)}{|g'(x_i)|}. \tag{3.29}$$

Thus, we have

$$\frac{1}{2\pi m}\int dte^{\frac{it(p^2-(p')^2)}{2m}}=\frac{1}{|p'|}(\delta(p-|p'|)+\delta(p+|p'|)). \tag{3.30}$$

Using the relation

$$\Theta(\alpha p)\Theta(\alpha p')(\delta(p-|p'|)+\delta(p+|p'|))=\delta(p-p'), \tag{3.31}$$

equation (3.26) becomes

$$\begin{aligned}\sum_{\alpha=\pm1}\int dt\,\langle p'|t,\alpha\rangle\langle t,\alpha|p\rangle&=\sum_{\alpha=\pm1}\frac{1}{2\pi m}\sqrt{|p|}\sqrt{|p'|}\Theta(\alpha p)\Theta(\alpha p')\int dt\,e^{\frac{it(p^2-(p')^2)}{2m}},\\&=\sqrt{|p|}\sqrt{|p|}\frac{1}{|p|}\delta(p-p'),\\&=\delta(p-p').\end{aligned}$$

Using the orthogonality relation $\langle p'|p\rangle=\delta(p-p')$, we identify the completeness relation for the eigenstates of the time operator:

$$\sum_{\alpha=\pm1}\int_{-\infty}^{\infty}dt\,|t,\alpha\rangle\langle t,\alpha|=\mathbb{1}. \tag{3.32}$$

Now, we are able to define the time POVM for the free particle[1]. For a time interval $\Delta t=(t_1,t_2)$, the operator $\mathbb{T}(\Delta t)$ is defined as the sum over all possible states of the free particle within the interval Δt between t_2 and t_1, such that

$$\mathbb{T}(\Delta t)=\sum_{\alpha=\pm1}\int_{t_1}^{t_2}dt\,|t,\alpha\rangle\langle t,\alpha|. \tag{3.33}$$

1 For more information about the time POVM, see [38].

It can be observed that when $t_1 \to -\infty$ and $t_2 \to \infty$, the completeness relation is recovered, i.e., $\mathbb{T} \to 1$. Within the POVM formalism, the probability of detecting the particle in the state $|\psi\rangle$ at $x = 0$ between the instants t_1 and t_2 is given by

$$P(\Delta t|x=0) = \langle\psi|\, \mathbb{T}(\Delta t)\, |\psi\rangle = \sum_{\alpha=\pm1} \int_{t_1}^{t_2} dt\, \langle\psi|t,\alpha\rangle \langle t,\alpha|\psi\rangle = \sum_{\alpha=\pm1} \int_{t_1}^{t_2} dt |\, \langle t,\alpha|\psi\rangle\, |^2. \tag{3.34}$$

We can identify the Kijowski probability distribution [39] as

$$\mathcal{T}(t) = \sum_{\alpha=\pm1} |\, \langle t,\alpha|\psi\rangle\, |^2, \tag{3.35}$$

or in the momentum representation

$$\mathcal{T}(t|x=0) = \sum_{\alpha=\pm1} \frac{1}{2\pi m} \int dpdp'\; \Theta(\alpha p)\Theta(\alpha p')\phi_\psi^*(p)\phi_\psi(p')\sqrt{|pp'|}e^{\frac{it(p^2-(p')^2)}{2m}}, \tag{3.36}$$

where $\phi_\psi(p)$ is the wave function of the state $|\psi\rangle$ in the momentum representation.

It is important to notice that the distribution $\mathcal{T}(t|x=0)$ admits $t \in \mathbb{R}$. However, the state $|\psi\rangle$ used to compute the Kijowski probability distribution is to be interpreted as a Schrödinger picture state prepared at an instant $t = \lambda$. In this case, only the values $t > \lambda$ are taken into account, since it does not make sense to be able to detect the particle before it was even prepared. But this gives a question: if $\lambda = 0$, how we can interpret the meaning of the negative values of time of arrival?

To circumvent this problem, we will use the interpretation proposed in [40]: we suppose that the particle was prepared in the far past $\lambda \to -\infty$ and have evolved without any perturbation to state $|\psi(t=0)\rangle$, which we have used to define the probabilities of time of arrival. Obviously, in an experiment we will be able to only detect positive times of arrival, but this gives a proper interpretation to the negative values of time in the theory.

3.2.2 Page-Wootters Mechanism

The Page-Wootters mechanism (PWM) [15, 41] was proposed in 1983 and has had a significant influence on the development of quantum gravity and discussions regarding time as an observable. In these works, the authors argue that time emerges from correlations (entanglement) between the system under observation and an external clock (for an extensive review see [42]).

In the PWM, time is defined as "what is shown in the clock", meaning that any dynamical system can be used to mark the passage of time. The most simple case of a quantum clock is the free particle, where time is seen as the position of the particle. It is important to point out that the physical definition of the quantum clock is not relevant, since one can consider the time Hilbert space $\mathcal{H}_T$ as an abstract space with no physical meaning.

The global Hilbert space is $\mathcal{H}_{TS} = \mathcal{H}_T \otimes \mathcal{H}_S$, where $\mathcal{H}_S$ is the Hilbert space of the system. For the time Hilbert space, it is introduced the position operator T and the conjugate momentum operator Ω, with $[T, \Omega] = i\hbar\mathbb{1}$, and the energy of the clock is associated with the operator Ω, which is a good approximation for massive and non-relativistic particles [43]. The fact that T represents the time operator which describes the evolution of a system can be enforced by imposing the following constraint equation, namely by requiring that the only states $|\Psi\rangle\rangle$ of the joint Hilbert space $\mathcal{H}_{TS}$ that represent physically relevant situations are the ones that satisfy

$$(\hbar\Omega \otimes \mathbb{1}_S + \mathbb{1}_T \otimes H)\,|\Psi\rangle\rangle = 0, \tag{3.37}$$

where $\mathbb{1}_T \otimes H$ is the Hamiltonian of the system acting on $\mathcal{H}_S$ and the notation of the state $|\Psi\rangle\rangle$ is used as a reminder that this state belongs to the bipartite space $\mathcal{H}_{TS}$. The equation (3.37) can be interpreted as the Wheeler-DeWitt equation [44], which have static eigenstates. However, the system and the clock evolve, in the sense that the correlations (entanglement) between system and clock track the system evolution. The solutions of (3.37) are

$$|\Psi\rangle\rangle = \int_{-\infty}^{\infty} d\omega\, |\omega\rangle\, |\psi(\omega)\rangle\,, \tag{3.38}$$

where $|\omega\rangle$ are the eigenstates of the operator Ω with eigenvalue ω and $|\psi(\omega)\rangle$ the Fourier transform of the system state $|\psi(t)\rangle$. Indeed, the solution of the equation (3.37) can be rewritten as

$$|\Psi\rangle\rangle = \int_{-\infty}^{\infty} dt\, |t\rangle\, |\psi(t)\rangle\,, \tag{3.39}$$

where $|t\rangle$ are the eigenstates of the operator T with eigenvalue t and $|\psi(t)\rangle$ is the eigenstate of the system. With the state (3.39), the equation (3.37) in the position representation becomes

$$\langle t|\,(\hbar\Omega \otimes \mathbb{1}_S + \mathbb{1}_T \otimes H)\,|\Psi\rangle\rangle = (-i\hbar\frac{\partial}{\partial t} + H)\,|\psi(t)\rangle = 0, \tag{3.40}$$

where the momentum operator is written in the position representation $\langle t|\,\Omega = (-i\frac{\partial}{\partial t})\,\langle t|$. This is clearly Schrödinger's equation for the system S that evolves with respect clock time t.

Before we finish this section, it is important to see that the Pauli objection do not apply to the time operator in the PWM. Differently from the Aharonov-Bohm approach of time observable, in the PWM the commutation relation for the time operator T and the Hamiltonian of the system H is $[T, H] = 0$, since the operators T and H do not act in the same Hilbert space. So, the time operator T can be self-adjoint and the Hamiltonian of the system H can have a lower bound, bypassing the Pauli objection.

3.3 Which Way Information

Niels Bohr, one of the most influential physicists of his time, proposed that in nature all things comes in pairs, such as space-time or position and momentum, and they cannot be observed simultaneously [45]. In modern quantum theory, this is applicable in the uncertainty principle and in the wave-particle duality, which is explained by what he called the complementary principle. A simple application of this concept can be seen in the double slit experiment.

In the double-slit experiment, an unpolarized light beam is directed toward a double-slit apparatus, with a film placed immediately behind the slits to record the final position of the light. An interference pattern is observed on the film, resulting from the diffraction of light, demonstrating its wave-like behavior. However, when a horizontal polarizer is placed in front of one slit and a vertical polarizer in front of the other, the film records two distinct points, indicating that the light exhibits particle-like behavior with a well-defined trajectory. According to Bohr's principle of complementarity, light cannot simultaneously exhibit both wave-like and particle-like behaviors. The observed behavior depends on the type of measurement performed.

Inspired by this, Englert [46] proposed that the information about the path that the particle took and the visibility of the interference pattern must satisfy the following inequality:

$$\mathcal{I}^2 + \mathcal{V}^2 \leq 1, \tag{3.41}$$

where $\mathcal{I}$ is associated with the path information, a particle behavior, and $\mathcal{V}$ is associated with the visibility of the interference pattern, a wave behavior. The equation (3.41) becomes an equality when the ensemble in the experiment is pure. What is interesting about this inequality is the possibility of having both wave and particle qualities partially, but always respecting the upper bound.

The quantity $\mathcal{I}$ represents the amount of information available about the path taken by the particle in an interferometer or, equivalently, the information about which slit the light beam passed through in the double-slit experiment. The visibility $\mathcal{V}$ of the interference pattern is defined as

$$\mathcal{V} = \frac{I_{max} - I_{min}}{I_{max} + I_{min}}, \tag{3.42}$$

where I_{max} is the maximum intensity of the interference pattern and I_{min} is the minimum intensity. For pure ensembles, the amount of which-way information $\mathcal{I}$ can be determined by the relation $\mathcal{I} = \sqrt{1 - \mathcal{V}^2}$

In the next section, an insightful application of this concept to the Mach-Zehnder interferometer will be presented. It will be shown that, to create which-way information, it is necessary to entangle the spatial modes of the system with an additional degree of freedom, such as the polarization of light.

3.3.1 Mach-Zehnder Interferometer

The Mach-Zehnder interferometer was proposed in the 19th century to study the influence of gas compression on the refractive index [47]. The interferometer can be constructed as follows: initially, a beam of unpolarized photons propagates along the x-direction. The beam then encounters a beam splitter, BS_1, which divides it into two paths, A and B. These paths are reflected by mirrors, M_A and M_B, respectively, and subsequently recombined at a second beam splitter, BS_2. The resulting beams are detected by two detectors, D_x and D_y. Two variations of this interferometer will be discussed: one where the photons are initially separated by a BS_1 (Figure 4) and another where the photons are initially separated by a polarizing beam splitter PBS Figure 5).

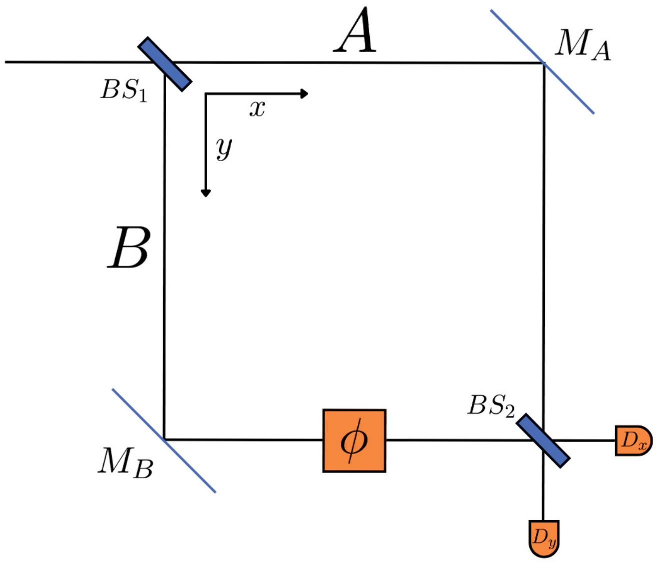


Figure 4 – Diagram of the Mach-Zehnder interferometer. BS_1 is the first beam splitter, M_A and M_B are mirrors, ϕ is the phase shifter and BS_2 is the second beam splitter.

Photons traveling in the horizontal direction (x-direction) are defined to be in the spatial mode $|x\rangle$, while those traveling in the vertical direction are in the spatial mode $|y\rangle$ (y-direction). The action of the beam splitter is represented by the following matrix:

$$BS = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \tag{3.43}$$

and the action of the mirrors are defined as

$$\begin{cases} M_A : |x\rangle \to i\,|y\rangle\,, \\ M_B : |y\rangle \to i\,|x\rangle\,. \end{cases} \tag{3.44}$$

The phase shifter ϕ will apply a phase into the spacial mode $|x\rangle$, such that $\phi\,|x\rangle = e^{i\phi}\,|x\rangle$. If the initial state of the photon is given by the spatial mode $|x\rangle$, then the evolution of the photon for the first configuration (Figure 4) of the Mach-Zander interferometer is

$$|\psi_{in}\rangle = |x\rangle \xrightarrow{BS_1, M_A, M_B} \frac{i\,|y\rangle - |x\rangle}{\sqrt{2}} \xrightarrow{\phi} \frac{i\,|y\rangle - e^{i\phi}\,|x\rangle}{\sqrt{2}} \xrightarrow{BS_2} \frac{i\,|y\rangle\,(1 - e^{i\phi}) - |x\rangle\,(1 + e^{i\phi})}{2}, \tag{3.45}$$

or

$$|\psi_{out}\rangle = e^{i\phi}[\sin(\phi/2)\,|y\rangle - \cos(\phi/2)\,|x\rangle]. \tag{3.46}$$

The probability of detection for each path is

$$P(x) = \mathrm{Tr}[D_x \rho] = \cos^2(\phi/2), \tag{3.47}$$

$$P(y) = \mathrm{Tr}[D_y \rho] = \sin^2(\phi/2), \tag{3.48}$$

here $\rho = |\psi_{out}\rangle\,\langle\psi_{out}|$, $D_x = |x\rangle\,\langle x|$, and $D_y = |y\rangle\,\langle y|$. In this type of interferometer, an interference pattern, as observed in the double-slit experiment, is not directly visible. However, the intensity of the interference can be quantified by the number of clicks registered by one of the detectors, such that

$$I(\phi) = \mathrm{Tr}[D_x \rho] = \cos^2(\phi/2). \tag{3.49}$$

Then, the visibility $\mathcal{V}$ becomes

$$\mathcal{V} = \frac{\max(\cos^2(\phi/2)) - \min(\cos^2(\phi/2))}{\max(\cos^2(\phi/2)) + \min(\cos^2(\phi/2))} = 1. \tag{3.50}$$

So, the which-way information for this case is $\mathcal{I} = \sqrt{1 - \mathcal{V}^2} = 0$, where we took into account that the ensemble is pure. This means that the photon behave purely as wave independently from the phase ϕ, and we cannot predict the path each photon took in the interferometer.

The experiment is now repeated, but instead of using a beam splitter initially, a PBS is employed. This ensures that each path corresponds to a specific polarization. Specifically, photons in path A are horizontally polarized ($|H\rangle$), while photons in path B are vertically polarized ($|V\rangle$). Using the same initial state $|\psi_{in}\rangle = |x\rangle$, the time evolution of the second Mach-Zehnder interferometer (Figure 5) is

$$\begin{aligned} |\psi_{in}\rangle = |x\rangle &\xrightarrow{PBS} \frac{1}{\sqrt{2}}(|x\rangle\,|H\rangle + i\,|y\rangle\,|V\rangle) \xrightarrow{M_A, M_B, \phi} \frac{1}{\sqrt{2}}(i\,|y\rangle\,|H\rangle - e^{i\phi}\,|x\rangle\,|V\rangle) \\ &\xrightarrow{BS_2} \frac{1}{2}[i\,|y\rangle\,(|H\rangle - e^{i\phi}\,|V\rangle) - |x\rangle\,(|H\rangle + e^{i\phi}\,|V\rangle). \end{aligned} \tag{3.51}$$

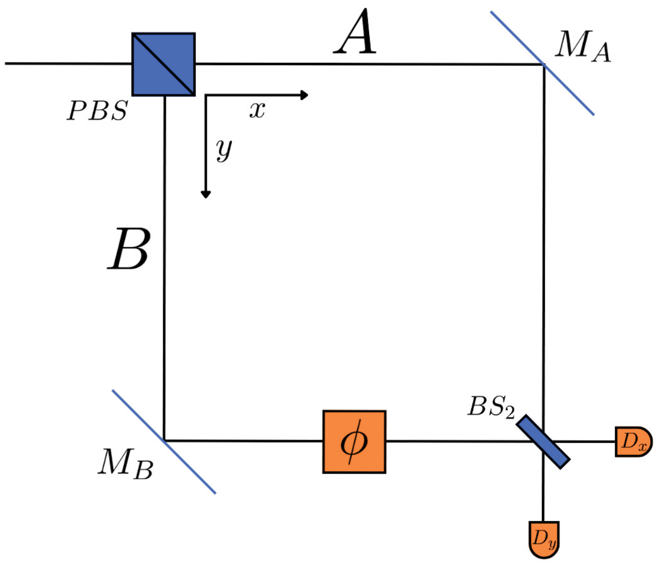


Figure 5 – Diagram of the Mach-Zehnder interferometer. PBS is the polarizing beam splitter, M_A and M_B are mirrors, ϕ is the phase shifter and BS_2 is the second beam splitter.

The final state after the second beam splitter BS_2 is

$$|\psi_{out}\rangle = \frac{1}{2}[i\,|y\rangle\,(|H\rangle - e^{i\phi}\,|V\rangle) - |x\rangle\,(|H\rangle + e^{i\phi}\,|V\rangle)], \tag{3.52}$$

with the following detection probabilities:

$$P(x) = \mathrm{Tr}[D_x \otimes \mathbb{1}_P \rho] = \frac{1}{2}, \tag{3.53}$$

$$P(y) = \mathrm{Tr}[D_y \otimes \mathbb{1}_P \rho] = \frac{1}{2}, \tag{3.54}$$

where $\mathbb{1}_P$ is the identity matrix for the Hilbert space of the polarization states. In this case, we do not observe any interference. Indeed, the visibility $\mathcal{V}$ for this experiment is

$$\mathcal{V} = \frac{\max(1/2) - \min(1/2)}{\max(1/2) + \min(1/2)} = 0, \tag{3.55}$$

and the which way information is $\mathcal{I} = 1$. We can see that, since the spatial modes of the photon are entangled with its own linear polarization, the photon are marked for each path of the interferometer, making it behave purely as a particle and destroying the visibility of the interference.

An important conclusion drawn from this experiment is that the creation of which-way information requires the entanglement of the spatial modes of the interferometer with states associated with the paths taken by the system. In this case, the spatial modes were entangled with the linear polarization of light, where each polarization was correlated with a distinct path.

Indeed, in the first case of the Mach-Zehnder interferometer the beam of light is unpolarized. Then, when we take into account the polarization of the photon, the final state can be written as

$$|\psi_{out}\rangle = \frac{e^{i\phi}}{\sqrt{2}}[\sin(\phi/2)\,|y\rangle - \cos(\phi/2)\,|x\rangle](|H\rangle + |V\rangle). \tag{3.56}$$

Since the states are separable, it is easy to see that the degrees of freedom are not entangled. However, on the second configuration, the final state is

$$|\psi_{out}\rangle = \frac{1}{2}[i\,|y\rangle\,(|H\rangle - e^{i\phi}\,|V\rangle) - |x\rangle\,(|H\rangle + e^{i\phi}\,|V\rangle)]. \tag{3.57}$$

In this case, the states of the spatial modes and linear polarization are not separable, meaning that the degrees of freedom are entangled.

3.4 Can Time Mark Photons?

In the previous sections, we have presented different approaches to time observables and demonstrated that the creation of which-way information destroys the interference pattern in interferometers. We are now ready to pose the central question of this chapter: Is a difference in time of flight sufficient to generate which-way information?

If time is indeed an observable, then it represents a degree of freedom. This implies that, in interferometers where each path has a different time of flight, the states corresponding to different time intervals should become entangled with the spatial modes of the photons, thereby generating which-way information and destroying the interference pattern.

To address this question, we will present an interferometer in which each path has a distinct time of flight. Subsequently, we will conduct a theoretical discussion of the results observed in the experiment.

3.4.1 Fizeau Interferometer

The Fizeau experiment was first introduced by Fizeau in 1851 [48], later refined by Michelson and Morley in 1886 [49] and reproduced by Zeeman in 1914 [50]. It played an important role in demonstrating that light does not obey the Galilean transformation between two moving reference frames. Years later, this inspired Lorentz to describe the light Doppler effect and, consequently, Einstein proposal of the special theory of relativity.

The Fizeau interferometer can be defined as follows: first, a light beam is generated at point S and divided into two beams by a lens at point L (figure 6). These beams are then collimated at point E by two slits, O_1 and O_2. Next, the beam passing through slit O_1 travels through tube A_1, where water is moving in the same direction as the light beam, while the beam passing through slit O_2 travels through tube A_2, where water is moving in the opposite direction. After passing through the tubes, the beams are recombined by the lens at point L' and reflected by the mirror at point m, forcing the beams to propagate through the tubes they have not yet traversed. This is done to minimize errors caused by potential inhomogeneities in the water flow and pressure. Finally, the beams collapse at surface S' positioned in G, where we can observe the interference pattern.

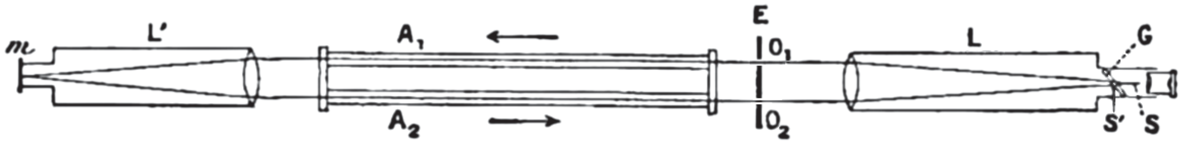


Figure 6 – Diagram of the Fizeau experiment. Picture took from [48].

At first glance, the speed of light by a Galilean transformation in each tube is

$$w_{\pm} = \frac{c_0}{n} \pm v, \tag{3.58}$$

with c_0 as the speed of light in vacuum, n is the refractive index of the water and v the velocity of the water in the laboratory reference frame. The plus or minus sign depends if the light travel in the same or opposite direction of the water current. But this experiment showed that the speed of light in each tube was given by

$$w_{\pm} = \frac{c_0}{n} \pm v\left(1 - \frac{1}{n^2}\right). \tag{3.59}$$

With the special theory of relativity, we can demonstrate the result obtained by Fizeau. The velocity-addition formula is given by

$$w = \frac{u+v}{1+(\frac{uv}{c_0^2})}, \tag{3.60}$$

where u is the velocity of the object in the rest frame, v is the velocity of the moving frame and w is the velocity of the object for the moving frame. Applying this formula to the case of the Fizeau experiment

$$w = \frac{\frac{c_0}{n}+v}{1+\frac{\frac{c_0}{n}v}{c_0^2}} = \frac{\frac{c_0}{n}+v}{1+\frac{v}{c_0 n}}. \tag{3.61}$$

Writing the difference of velocities w and $\frac{c_0}{n}$

$$w - \frac{c_0}{n} = \frac{\frac{c_0}{n}+v}{1+\frac{v}{c_0 n}} - \frac{c_0}{n} = \frac{\frac{c_0}{n}+v-\frac{c_0}{n}(1+\frac{v}{c_0 n})}{1+\frac{v}{c_0 n}} = \frac{v(1-\frac{1}{n^2})}{1+\frac{v}{c_o n}} \tag{3.62}$$

Defining that the velocity of the fluid v is much smaller that the speed of light $\frac{c_0}{n}$,

$$w - \frac{c_0}{n} \approx v\left(1 - \frac{1}{n^2}\right). \tag{3.63}$$

Then, the speed of light in the cases where the light propagates in the same direction as the fluid current (w_+) and in the opposite direction (w_-) is

$$w_\pm = \frac{c_0}{n} \pm v\left(1 - \frac{1}{n^2}\right), \tag{3.64}$$

which is identical to what Fizeau saw in (3.59). It is important to say that, since the first postulate of special relativity defines that the speed of light is constant in all referentials, in this case what changes for each tube is the time of flight and $w_\pm$ represents the effective speed of light. In 1898, Lorentz added the dispersion contribution, giving the final definition of the Fizeau drag coefficient [51]

$$w_\pm = \frac{c_0}{n} \pm v\left(1 - \frac{1}{n^2} - \frac{\lambda}{n}\frac{dn}{d\lambda}\right), \tag{3.65}$$

with λ as the wavelength of the light used in the experiment.

After the first application of the experiment by Fizeau, Michelson and Morley improved the experimental procedure with technological advancements and then Zeeman reproduced the Michelson and Morley experimental apparatus with light with different wavelengths to confirm the dispersion contribution proposed by Lorentz. In the Zeeman case, he initially made the experiment with the water current in the same direction for both paths, generating a interference pattern in the film. Then, he positioned a wire in front of the interference pattern so he could use it as a parameter. After this, he made the water flow in different directions in each path and saw the displacement of the interference pattern. The results are in Figure 7.

The interference pattern in the case (a) is caused by the differences in the optical paths of the interferometer. The displacement of the fringes in the case (b) is caused by the phase associated with the different time of flight of the optical paths. Indeed, the time of flight for each path is

$$t_+ = \frac{2L}{w_+} = \frac{1}{10^8 - 10^{-3}}\mathrm{s}, \tag{3.66}$$

$$t_- = \frac{2L}{w_-} = \frac{1}{10^8 + 10^{-3}}\mathrm{s}, \tag{3.67}$$

where L is the length of the tubes. The difference of time of flight between the tubes is

$$\delta_t = \frac{4Lvn^2}{c^2}\left(1 - \frac{1}{n^2} - \frac{\omega}{n}\frac{dn}{d\omega}\right) \approx 10^{-19}\mathrm{s}, \tag{3.68}$$

and the lateral displacement of the fringes is given by

$$\Delta = \frac{\delta_t c}{\lambda} = \frac{4Lvn^2}{c\lambda}\left(1 - \frac{1}{n^2} - \frac{\omega}{n}\frac{dn}{d\omega}\right). \tag{3.69}$$

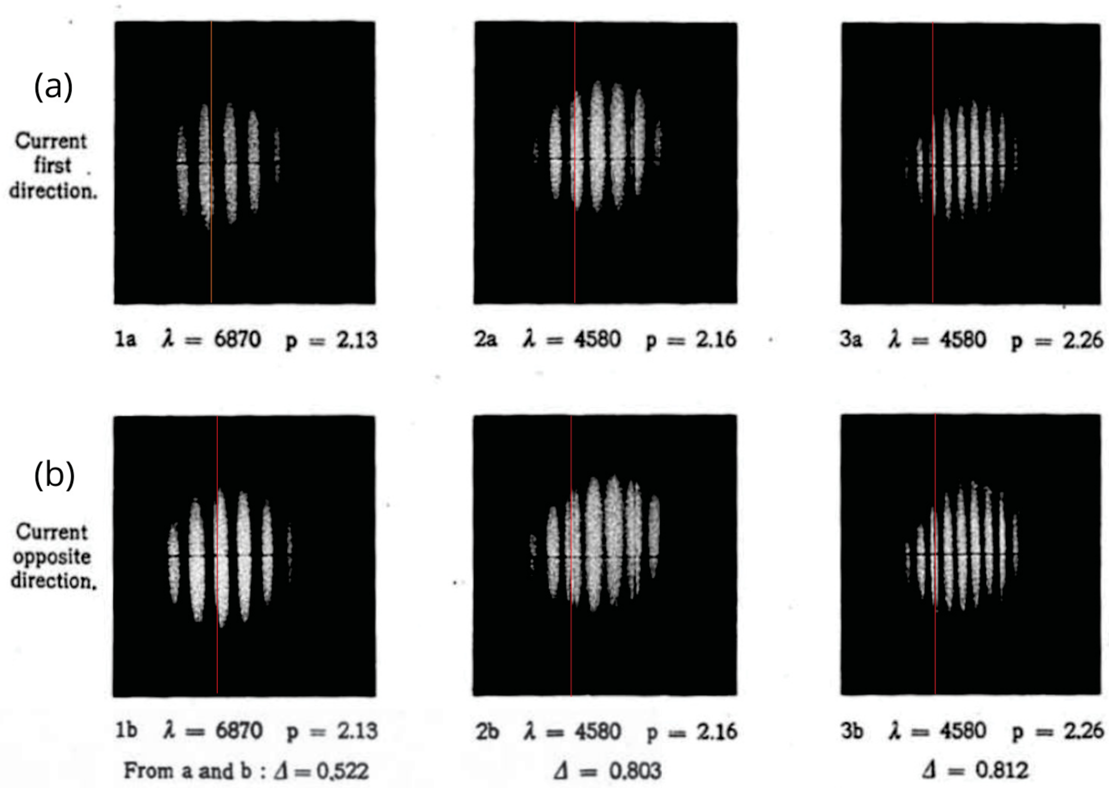


Figure 7 – Interference pattern for the water current in the same direction in each path (a) and for the water current in different directions (b). λ is the wavelength of the light in Å, p in the water pressure in kg/cm^2 and Δ is the displacement of the fringes. The red line represents the position of the wire. Figure taken from [50].

The lateral displacement Δ is caused by the increase in the relative phase between the light beams, which moves the interference pattern. The lateral displacement is then measured, and the Fizeau drag coefficient is experimentally determined.

3.4.2 Entanglement with Time

In the Fizeau experiment, we saw that the difference of time of flight of each path was capable to generate lateral displacement of the fringes of the interference pattern. In the theoretical description of the experiment, time is defined as a parameter. If we take into account the quantum description of time given by the time operator, we would expect the state of the system to be given by

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|x\rangle\,|t_+\rangle + |y\rangle\,|t_-\rangle), \tag{3.70}$$

where $|x\rangle$ and $|y\rangle$ are the spatial modes of the interferometer, $|t_+\rangle$ and $|t_-\rangle$ are the states of time of flight for each tube. In this case, since the time of travel is entangled with the spatial modes, time should works as which-way information and so we expected that the visibility of the interference pattern to be reduced. But that is not what we see in the Fizeau experiment, suggesting that the spatial modes of the interferometer are not entangled with time, or

$$|\psi\rangle \approx \frac{1}{\sqrt{2}}(|x\rangle + |y\rangle)\,|t\rangle\,. \tag{3.71}$$

A criterion to determine entanglement in bipartite pure states is by the linear entropy of the reduced state [52]

$$E(\rho_{TS}) = S_L(\rho_S) = 1 - \mathrm{Tr}[\rho_S^2]. \tag{3.72}$$

If the reduced state ρ_S is pure, then the linear entropy is $S_L(\rho_S) = 0$. This means that it is possible to assert if the subsystems are entangled based on the purity of the reduced state. The total state of the system is

$$\begin{aligned} 2\rho_{TS} = 2\,|\psi\rangle\,\langle\psi| = |x\rangle\,\langle x| \otimes |t_+\rangle\,\langle t_+| + |y\rangle\,\langle y| \otimes |t_-\rangle\,\langle t_-| + \\ |x\rangle\,\langle y| \otimes |t_+\rangle\,\langle t_-| + |y\rangle\,\langle x| \otimes |t_-\rangle\,\langle t_+|\,. \end{aligned} \tag{3.73}$$

The reduced state is

$$2\mathrm{Tr}_T[\rho_{TS}] = 2\rho_S = |x\rangle\,\langle x| + |y\rangle\,\langle y| + |x\rangle\,\langle y|\,\langle t_+|t_-\rangle + |y\rangle\,\langle x|\,\langle t_-|t_+\rangle\,. \tag{3.74}$$

The purity of the reduced state ρ_S will be

$$4\mathrm{Tr}[\rho_S^2] = 2 + 2|\,\langle t_+|t_-\rangle\,|^2. \tag{3.75}$$

or

$$\mathrm{Tr}[\rho_S^2] = \frac{1 + |\,\langle t_+|t_-\rangle\,|^2}{2}. \tag{3.76}$$

Supposing we can rewrite the term $|\,\langle t_+|t_-\rangle\,|^2$ as Gaussian wave packets, such that

$$|\,\langle t_+|t_-\rangle\,|^2 = \left|\int d\tau\,\langle t_+|\tau\rangle\,\langle\tau|t_-\rangle\right|^2 \propto \left|\exp\left\{-\frac{(t_- - t_+)^2}{8\Delta T^2}\right\}\right|^2, \tag{3.77}$$

where ΔT is the width of the wave packets and $|\tau\rangle$ are the eigenstates of a time operator. By the exponential in (3.77), we can see that, since the spatial modes are not entangled with the states of the time of flight, the argument of the exponential must go to zero, making the state ρ_S to be pure. The problem is that the theoretical descriptions of time observables in literature do not give us the magnitude of the dispersion of the time operator, precluding the advance of this theoretical discussion. We conclude that the Fizeau interferometer has the potential to determine if time is an observable in the theory of quantum mechanics, but the parameters of the experiment must be manipulated in a way that the quantum behavior of time is possible to be observed.

CHAPTER 4

Irrealism and Macrorealism

4.1 EPR and Elements of Reality

In 1935, Einstein, Podolsky and Rosen published an article entitled "Can Quantum-Mechanical Description of Physical Reality be Considered Complete" [5]. In this classical work, the authors discuss what it means to a theory to be correct and complete, and also define something called "element of reality".

The authors argue that a physical theory is said to be correct if the theory agrees with the experimental results, which is a satisfactory definition not only for physical theories, but all natural sciences.

They define what it means to a theory to be complete and what is an element of reality as follows

- *Complete*: Every element of reality must have a counterpart in the physical theory.
- *Element of Reality*: If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity.

In the original work, the authors make an example with continuum variables. For the sake of simplicity, we will make some examples using qubits. For a particle in the positive eigenstate of S_z, $|\psi\rangle = |z,+\rangle$, the probability of finding the particle in the $|z,+\rangle$ will be $P_z(+) = 1$. Now, if we have a state of the form $|\psi\rangle = \frac{1}{\sqrt{2}}(|z,+\rangle + |z,-\rangle)$, the probability of finding the particle in the same state is $P_z(+) = 1/2$. As we can see from these probabilities, there are cases in quantum mechanics where a physical quantity can represent an element of reality. But does this mean the theory is complete? Assuming the first system $|\psi\rangle = |z, +\rangle$, the probability of finding the state in the positive S_x eigenstate is $P_x(+) = 1/2$, which is different from unity. This suggest that theirs definition of a complete theory is not allowed in quantum mechanics.

This result exemplifies the non-commuting nature of spins in different directions. In the sense of EPR, the spin in two different directions cannot have elements of reality simultaneously. From this, the authors define two alternatives: (1) *the description of the physical reality given by the wave function is incomplete*, or (2) *physical quantities assigned to incompatible observables cannot have simultaneous reality*.

The theory of quantum mechanics presumes that (1) is false and, therefore, (2) must be true. However, the authors show in a thought experiment that it is possible for (2) be false, and by consequence (1) be true. We will show the experiment proposed by D. Bohm [53] using a system with a discrete spectrum of outcomes instead of the continuous one used by EPR.

A source creates a pair of entangled electron-positron, where one of them is given to Bob, in the lab B, and the other to Alice, in lab A. The labs are space-like separated. The state of this pair will be a singlet state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+, z\rangle_A |-, z\rangle_B - |-, z\rangle_A |+, z\rangle_B), \tag{4.1}$$

or

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+, x\rangle_A |-, x\rangle_B - |-, x\rangle_A |+, x\rangle_B), \tag{4.2}$$

where we used the identities of S_z eigenstates as a superposition of S_z eigenstates. If Alice measures the S_x component with the +1 outcome ($|+, z\rangle_A$), then Bob will observe only the -1 outcome ($|-, z\rangle_B$), making S_z an element of reality for Bob. If the same is done for S_x by Alice, then Bob's qubit will be in a well-defined state, and S_x will also be an element of reality. As the labs A and B are space-like separated, the measurements made by Alice should not be correlated with the ones made by Bob, in such a way that we need to admit both wave functions resulting from the possible measurements made by Alice as possible for Bob. From this, the authors say that S_z and S_x represent simultaneously elements of reality for Bob, which makes (2) false, and so (1) true.

The authors hoped that this paradox could be resolved in a way that quantum mechanics would satisfy the local causality hypotheses, i.e. the reality of a physical quantity could not be changed by space-like separated events. This inspired physicist to propose the "theory of hidden variables", which, as we will see in the following section, is incompatible with quantum mechanics.

4.1.1 Bell's Theorem

In 1964, Bell published an article entitled "On the Einstein Podolsky Rosen Paradox" [9], in which he demonstrated the incompatibility of quantum mechanics with the theory of local hidden variables. As previously discussed, if quantum mechanics is assumed to be a local theory, it must also be considered incomplete. To address this incompleteness, some physicists proposed the existence of local hidden variables, which would account for the correlations observed in measurements of space-like separated systems.

A source creates two entangled qubits that are given each one to Alice and Bob, who resides in space-like separated laboratories as in Figure 8. Alice make numerous measurements of the physical quantity A with possible outcomes a and Bob make measurements of the physical quantity B with outcomes b. The outcomes may vary for each iteration. After the experiments, they will be able to compute the probability distribution $p(a, b|A, B)$ and show that this distribution is not factorizable $p(a, b|A, B) \neq p(a|A)p(b|B)$, meaning that the outcomes $\{a, b\}$ are statistically correlated.

Assuming that quantum mechanics is a local theory, there should not have any correlation between the events, since Alice and Bob cannot instantaneously communicate with each other. For this, physicists proposed the existence of a local hidden variable λ which was capable to make the probability of the outcomes independent from the events, such that

$$p(a, b|A, B) = \int d\lambda p(\lambda)p(a, b|A, B, \lambda), \tag{4.3}$$

where $p(\lambda)$ is the probability distribution of the hidden variable λ and the joint probability on the left side of the equation is $p(a, b|A, B, \lambda) = p(a|b, A, B, \lambda)p(b|A, B, \lambda)$, meaning that the statistical correlation could be undone by the specification of the variable λ.

Now, we will make some assumptions so that the equation (4.3) is satisfied by any deterministic and local theory. Cavalcanti and Wiseman [54] say that a system is deterministic[1] if and only if $p(a, b|A, B, \lambda) \in \{0, 1\}$, $a \equiv a(A, B, \lambda)$ and $b \equiv b(A, B, \lambda)$. A consequence from this is the independence of the outcomes $\{a, b\}$ from each other, such that $p(a|b, A, B, \lambda) = p(a|A, B, \lambda)$ and vice versa. If the theory is local, the possible outcomes of the observables A and B should depend only on events occurring in the vicinities of the laboratories. Thus, the conditional probabilities of the outcomes becomes $p(a|A, B, \lambda) = p(a|A, \lambda)$ and $p(b|A, B, \lambda) = p(b|B, \lambda)$. With this, equation (4.3) can be rewritten as

$$p(a, b|A, B) = \int d\lambda p(\lambda)p(a|A, \lambda)p(b|B, \lambda). \tag{4.4}$$

[1] In this case, determinism and realism are the same concept, meaning that the outcomes of the observables are well established even before any measurement.

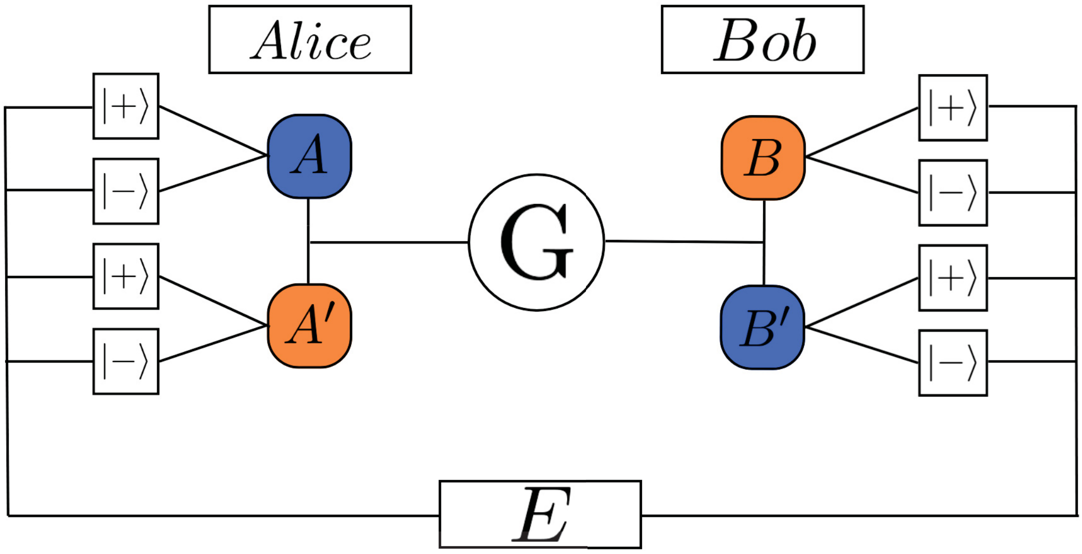


Figure 8 – Diagram of the CHSH experiment. Two entangled qubits are generated in G. Then, they are separated between two labs, Alice and Bob. In these labs, two measurements are made in each: A and A' in Alice's lab, and B and B' in Bob's lab. The probabilities are sent to an external agent E, who calculates the correlation functions for those probabilities.

A way to assert whether the system satisfies the condition in (4.4), is by the Clauser-Horne-Shimony-Holt (CHSH) inequality [10]. Given that the correlation function between two observables A and B is

$$C_{AB} = \langle A \otimes B \rangle = \int_a \int_b da\ db\ p(a, b|A, B)ab. \tag{4.5}$$

If the system is deterministic and local

$$C_{AB} = \int_\lambda d\lambda\ p(\lambda) \int_a da\ p(a|A, \lambda)a \int_b db\ p(b|B, \lambda)b, \tag{4.6}$$

or

$$C_{AB} = \int_\lambda d\lambda\ p(\lambda)\langle A\rangle_\lambda \langle B\rangle_\lambda, \tag{4.7}$$

and defining that both Alice and Bob may have two other possible observables A' and B', respectively, we define a quantity called correlator S:

$$S = C_{AB} + C_{A'B} + C_{AB'} - C_{A'B'}. \tag{4.8}$$

Substituting (4.7) in S

$$S = \int_\lambda d\lambda\ p(\lambda)[\langle A\rangle_\lambda(\langle B\rangle_\lambda + \langle B'\rangle_\lambda) + \langle A'\rangle_\lambda(\langle B\rangle_\lambda - \langle B'\rangle_\lambda)]. \tag{4.9}$$

As we said previously, the system is constituted by qubits, meanings that the possible outcomes of the observables are $+1$ or -1. With this, it is possible to demonstrate that any system that satisfies the conditions of determinism and locality should satisfy the following inequality

$$C_{AB} + C_{A'B} + C_{AB'} - C_{A'B'} \leq 2. \tag{4.10}$$

Let us make an example to elucidate how quantum mechanics violates the inequality. Suppose the system is in the singlet state in (4.1). The correlation functions for two spins $A = \hat{a} \cdot \vec{\sigma}$ and $B = \hat{b} \cdot \vec{\sigma}$ is $\langle AB \rangle = -\hat{a} \cdot \hat{b}$. If Alice measures the qubit in $\hat{a} = \hat{x}$ and $\hat{a}' = \hat{y}$ directions, and Bob measures in $\hat{b} = \frac{1}{\sqrt{2}}(\hat{x} + \hat{y})$ and $\hat{b}' = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y})$ directions, the correlation functions will be $\langle ab \rangle = \langle ab' \rangle = \langle a'b \rangle = \frac{1}{\sqrt{2}}$ and $\langle a'b' \rangle = -\frac{1}{\sqrt{2}}$. The correlator S will be $S = 2\sqrt{2}$, which violates the upper bound of the CHSH inequality. This implies that quantum mechanics violates the definitions of determinism and locality.

Numerous experiments with loopholes [55, 56] and without loopholes [57–59] have shown the violation of the CHSH inequalities, making it a cornerstone in the study of the foundations of quantum mechanics.

4.2 Irrealism

In 2015, Bilobran and Angelo (BA) published a paper entitled "A Measure of Physical Reality" [12], in which they proposed a new definition of elements of reality and also defined a quantity called Irreality. Their new definition has been proven to be more advantageous than the one proposed by EPR, as it can take into account mixed states.

We consider two laboratories, A and B, as illustrated in Figure 9. In the first laboratory, the state of a system is prepared, and quantum state tomography is performed by making numerous observations of the system. This allows for the reconstruction of the state as $\rho \in \mathcal{H}_T = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \cdots \otimes \mathcal{H}_N$. In the second laboratory, a system is prepared, and an external agent performs numerous non-revealed observations of a physical quantity A, where $A = \sum_n a_n \Lambda_{a_n}$. Following this, quantum state tomography is performed, resulting in the following completely positive trace-preserving (CPTP) map:

$$\Phi_A(\rho) = \sum_n \Lambda_{a_n} \rho \Lambda_{a_n} = \sum_n p(a_n) \Lambda_{a_n} \otimes \frac{\mathrm{Tr}_A[\Lambda_{a_n} \rho \Lambda_{a_n}]}{p(a_n)}, \tag{4.11}$$

where $p(a_n) = \mathrm{Tr}[\Lambda_{a_n} \rho]$ is the probability of the external agent obtaining the outcome a_n, and $\mathrm{Tr}_A[\Lambda_{a_n} \rho \Lambda_{a_n}]/p(a_n)$ is the part of the state that remains untouched by the external agent.

With this, the authors propose a new definition for elements of reality:

- *BA element of reality*: An observable $A = \sum_n a_n \Lambda_{a_n}$, with projectors $\Lambda_{a_n} = |a_n\rangle \langle a_n|$ acting on $\mathcal{H}_A$, is real for a preparation $\rho \in \mathcal{H}_T = \mathcal{H}_A \otimes \mathcal{H}_B \otimes ... \otimes \mathcal{H}_N$ if and only if

$$\rho = \Phi_A(\rho). \tag{4.12}$$

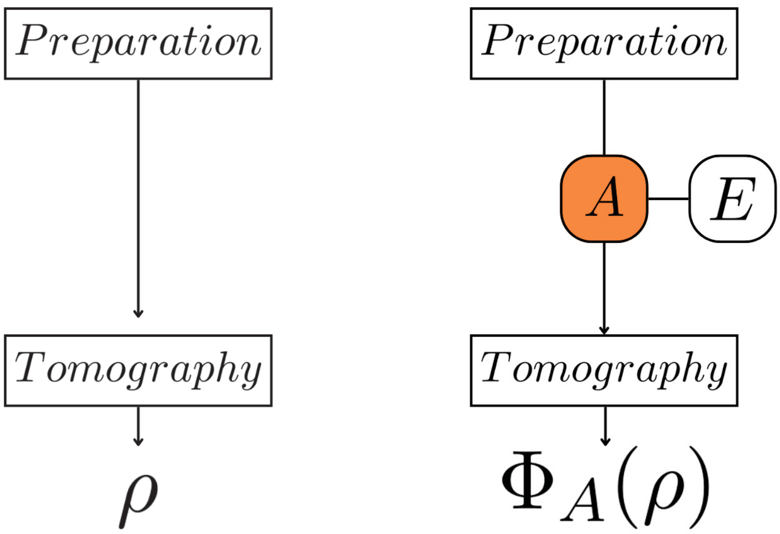


Figure 9 – Diagram of the construction of the map. On the left, numerous states are prepared and subjected to quantum state tomography, resulting in the reconstruction of the state ρ. On the right, numerous states are also prepared, but an external agent E performs non-revealed measurements of the observable A on the system. Subsequently, the system undergoes quantum state tomography, and the state is reconstructed as the map $\Phi_A(\rho)$. If $\Phi_A(\rho) = \rho$, then the observable measured by the external agent represents an element of reality.

To gain a better understanding of this definition, let us propose some examples. For a pure state $\rho = |a_n\rangle\langle a_n|$, the state after a non-revealed measurement becomes

$$\Phi_A(\rho) = \sum_n \Lambda_{a_n} |a_n\rangle\langle a_n| \Lambda_{a_n} = \rho, \tag{4.13}$$

indicating that A is a BA element of reality. Since the state $\rho = |a_n\rangle\langle a_n|$ is an eigenstate of the operator A, it is also an EPR element of reality. Now, if we have a pure state like

$$\rho' = \frac{1}{2}(|a_n\rangle\langle a_n| + |a_m\rangle\langle a_m| + |a_n\rangle\langle a_m| + |a_m\rangle\langle a_n|), \tag{4.14}$$

the map becomes $\Phi_A(\rho') = \frac{1}{2}(|a_n\rangle\langle a_n| + |a_m\rangle\langle a_m|)$. In this case, the observable A do not represent an BA element of reality but it is an EPR element of reality, since, again, the state ρ' represents an eigenstate of the operator A. Finally, for a mixed state $\rho'' = \frac{1}{2}(|a_n\rangle\langle a_n| + |a_m\rangle\langle a_m|)$, the map becomes

$$\Phi_A(\rho'') = \frac{1}{2}(|a_n\rangle\langle a_n| + |a_m\rangle\langle a_m|), \tag{4.15}$$

meaning that A is a BA element of reality for the state ρ''. In the original EPR paper, the authors do not discuss theirs definition of elements of reality for mixed states, maybe because the definition they proposed is only applicable to pure states.

It is interesting to notice that non-revealed measurements do not change a maximally mixed state. Indeed, having $\rho_{mm} = \frac{\mathbb{1}_A}{d_A}$, then the map becomes

$$\Phi_A(\rho_{mm}) = \sum_n \Lambda_{a_n} \frac{\mathbb{1}_A}{d_A} \Lambda_{a_n} = \frac{1}{d_A} \sum_n \Lambda_{a_n} = \frac{\mathbb{1}_A}{d_A}, \tag{4.16}$$

where we have used the idempotent property of the projectors ($\Lambda_{a_n}^2 = \Lambda_{a_n}$) and the completeness relation. Another interesting property is that sequential maps of the same observable do not change the map:

$$\Phi_A(\Phi_A(\rho)) = \sum_n \sum_m \Lambda_{a_n} \Lambda_{a_m} \rho \Lambda_{a_n} \Lambda_{a_m} = \sum_n \Lambda_{a_n} \rho \Lambda_{a_n} = \Phi_A(\rho), \tag{4.17}$$

where we have used the property of pairwise orthogonality of the projectors ($\Lambda_{a_n} \Lambda_{a_m} = \delta_{nm} \Lambda_{a_n}$). Therefore, sequential maps of the same observable preserve the reality status of the state.

Following the definition of BA elements of reality, the authors define a quantifier for the irreality of an observable A:

$$\mathfrak{I}_A(\rho) := S(\Phi_A(\rho)) - S(\rho), \tag{4.18}$$

where $\mathfrak{I}_A(\rho)$ is the irreality of the observable A given the state ρ, and $S(\rho)$ is the von Neumann entropy of the state ρ. The irreality is equal to the relative entropy $S(\rho||\Phi_A(\rho)) = \mathrm{Tr}[\rho(\log(\rho) - \rho\log(\Phi_A(\rho)))]$ [60]. This means that the irreality $\mathfrak{I}_A(\rho)$ is nonnegative:

$$\mathfrak{I}_A(\rho) \geq 0, \tag{4.19}$$

and goes to zero if and only if (4.12) is satisfied.

4.2.1 Joint Irrealism

More recently, Caetano and Angelo (CA) [61] proposed the joint irrealism, which can be used to detect if two observables represent joint elements of reality. Suppose we do the same experiment made by BA, but this time we do two sequential non-revealed measurements of two different observables $A = \sum_n \Lambda_{a_n} \rho \Lambda_{a_n}$ and $B = \sum_m \Lambda_{b_m} \rho \Lambda_{b_m}$. In this case, the external agent will produce the following map

$$\Phi_{AB}(\rho) = \Phi_A \circ \Phi_B(\rho) = \sum_{n,m} \Lambda_{b_m} \Lambda_{a_n} \rho \Lambda_{a_n} \Lambda_{b_m}, \tag{4.20}$$

where $\Phi_A \circ \Phi_B(\rho)$ represents the sequential map of the observables A and B. Inspired by BA, CA proposed that two observables will be joint elements of reality for a state ρ if

$$\Phi_{AB}(\rho) = \Phi_{BA}(\rho) = \rho. \tag{4.21}$$

Whenever this condition is satisfied, we say that the observables A and B represent joint elements of reality for the system ρ. In addition, given that $\Phi_A(\rho) = \Phi_A(\Phi_A(\rho))$, when (4.21) is true $\Phi_A \circ \Phi_{AB}(\rho) = \Phi_A(\rho) = \Phi_{AB}(\rho) \rightarrow \Phi_A(\rho) = \rho$, which means that if two observables represent joint elements of reality, then they also are BA elements of reality individually.

Given this definition, the authors also define the Joint Irreality:

$$\mathfrak{I}_{AB}(\rho) = \frac{S(\Phi_{AB}(\rho)) + S(\Phi_{BA}(\rho))}{2} - S(\rho). \tag{4.22}$$

Since the von Neumann entropy is non-decreasing under CPTP maps, the joint irreality is always semi-positive and goes to zero only if (4.21) is true. To prove this, let's make some addition and subtraction of the entropies $S(\Phi_A(\rho))$ and $S(\Phi_B(\rho))$ in (4.22). Thus, the joint irreality becomes

$$\mathfrak{I}_{AB}(\rho) = \frac{\mathfrak{I}_A(\rho) + \mathfrak{I}_B(\rho) + \mathfrak{I}_B(\Phi_A(\rho)) + \mathfrak{I}_A(\Phi_B(\rho))}{2}. \tag{4.23}$$

The relative entropies in (4.23) are going to be zero only if their arguments are equal, such that $\rho = \Phi_A(\rho) = \Phi_B(\rho) = \Phi_{AB}(\rho) = \Phi_{BA}(\rho)$.

Another discussion the authors show in the same work is a comparison between the joint irreality for the singlet state and the definition of simultaneous elements of reality in the EPR paper. For two maximally incompatible observables $A = X$ and $B = \bar{X}$, the joint irreality becomes

$$\mathfrak{I}_{X,\bar{X}} = \log_a d - S(\rho), \tag{4.24}$$

where d is the dimension of the Hilbert space where the observable acts. For the two observables $A = \mathbb{1} \otimes \sigma_z$ and $B = \mathbb{1} \otimes \sigma_x$, the joint irreality for the singlet state $\rho = |\psi\rangle \langle\psi|$ where $|\psi\rangle$ is the state in (4.1) is

$$\mathfrak{I}_{\mathbb{1}\otimes\sigma_z,\mathbb{1}\otimes\sigma_x}(\rho) = \log_a 4. \tag{4.25}$$

The result in (4.25) is a completely different result from the EPR's approach, in which the observables σ_x and σ_y represented simultaneous elements of reality in Bob's laboratory.

4.3 Macrorealism

One of the most renowned thought experiments in quantum mechanics is Schrödinger's cat. In this experiment, a cat is placed inside a box containing a flask of poison, a hammer positioned to break the flask, a radioactive material, and a Geiger counter. If the Geiger counter detects radiation—indicating the decay of the radioactive material—the hammer is triggered, breaking the flask and killing the cat. However, since atomic decay is a probabilistic event, the state of the cat (whether dead or alive) can only be determined upon observation of the system. Prior to observation, the system must be described as being in a superposition of the states corresponding to a dead cat and an alive cat [62].

Schrödinger presented this experiment to demonstrate how absurd the wave function description of nature can be when applied to "macroscopically tangible and visible things". Inspired by this, Leggett and Garg proposed a definition of how macroscopic objects should behave and also a test to determine whether they do exhibit this behavior [11] (for an extensive review see [63]).

In 1985, Leggett and Garg published an article entitled "Quantum mechanics versus macroscopic realism: Is the flux there when nobody looks?", where they discuss the concept of "macrorealism". The authors define that a system is not macrorealistic if it violates at least one of the following assumptions:

- **A1.** *Macroscopic realism per se* : A macroscopic system with two or more macroscopically distinct states available to it will at all times be in one or the other of these states.
- **A2.** *Non Invasive Mensurability*: It is possible, in principle, to determine the state of the system with arbitrarily small perturbation on its subsequent dynamics.

In more recent discussions, some authors have introduce a third assumption [64]:

- **A3.** *Induction*: The outcome of a measurement on the system cannot be affected by what will or will not be measured on it later.

Following the assumptions, the authors define the Leggett-Garg inequalities (LGIs)

$$K_3 = C_{12} + C_{23} - C_{13} \leq 1, \tag{4.26}$$

$$K_4 = C_{12} + C_{23} + C_{34} - C_{14} \leq 2, \tag{4.27}$$

where $C_{ij} = \langle Q_i Q_j \rangle$ are the two times correlation functions and $Q_i = Q(t_i)$ is an observable in the Heisenberg picture in the instant t_i and $t_1 < t_2 < t_3 < t_4$. When the upper limit of the inequalities is violated, the system do not satisfy macrorealism.

For any theory that obeys **A1**-**3**, the Schrödinger cat must be dead or alive in every instant of time and the observation of the cat state do not interfere with the cat itself. So, the definition of macrorealism is in tune with our perception of the macroscopic world, but is in total disagreement with quantum mechanics.

Assumption **A3** reflects such basic notions about causality and the arrow of time, that it has been unchallenged in discussions about the LGIs. **A1** also satisfies our intuition about the macroscopic world, and has been accepted by many authors as a necessary assumption to the deduction of the LGIs. **A2**, on the other hand, can be a little more problematic when we try to make a more profound discussion.

It can be argued that **A2** agrees with **A1**, as the measurement of a system should only reveal a pre-existing property of a macroscopic state. However, this poses a challenge in quantum theory, where measurements are inherently invasive. To address this issue, Leggett and Garg introduced the concept of *negative measurements*. Suppose one aims to measure a macroscopic variable $Q = \pm 1$ by employing a detector that interacts exclusively with the state corresponding to $Q = +1$. In this scenario, the absence of a detector response allows one to infer the state of the system ($Q = -1$) without direct interaction. This approach enables the determination of the system's state in a non-invasive manner.

Another, more significant issue is that a stubborn macrorealistic can argue that it is impossible to formulate a scientific hypothesis assuming perfect measurements that do not influence the experimental outcome. This is known as the *clumsiness loophole* [65], and a stubborn macrorealistic can always invoke this argument to dismiss experimental results demonstrating violations of the LGIs. Despite numerous attempts to address the clumsiness loophole [66–70], it remains an unresolved challenge in the context of macrorealism.

The LGIs have been verified in numerous experiments [71–73] and have proven to be an excellent test for determining whether a system violates the assumptions of macrorealism.

4.4 Leggett-Garg Inequalities

Similarly to the approach used for the CHSH inequality, a demonstration of the LGI can be presented based on the assumptions of macrorealism. For a qubit with a given time evolution, sequential observations of its spin are made at different instants of time t_i and t_j, where $t_i < t_j$ (Figure 10). This process is repeated as many times as necessary. The joint probability of obtaining outcomes q_i in the first observation Q_i and q_j in the second observation Q_j is

$$p(q_i, q_j | Q_i, Q_j, \epsilon) = p(q_i | Q_i, Q_j, \epsilon) p(q_i | q_j, Q_i, Q_j, \epsilon), \tag{4.28}$$

where ϵ is hidden variable that represents a complete catalog specifying all properties of the outcomes q_i and q_j and is not influenced by the time evolution of the system [74]. By A1, the measurements should only reveal a pre-existing state, in a way that the possible outcomes q_i and q_j are independent from one another

$$p(q_i, q_j | Q_i, Q_j, \epsilon) = p(q_i | Q_i, Q_j, \epsilon) p(q_j | Q_i, Q_j, \epsilon). \tag{4.29}$$

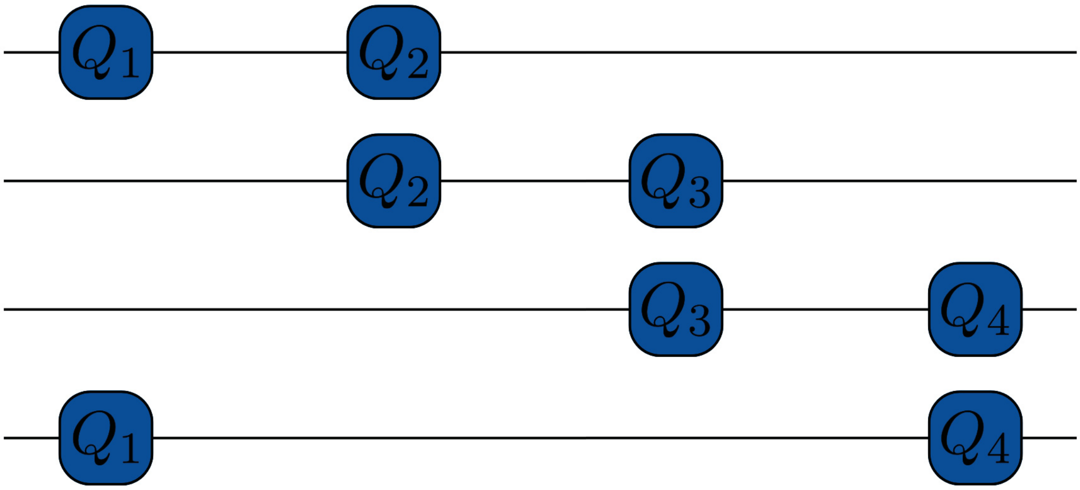


Figure 10 – Diagram of the LG experiment. The observations of the physical quantity Q is made in two different times t_i and t_j. Then, the joint probabilities for the possible outcomes are gathered an the correlation functions C_{ij} are constructed. This process is repeated four times for different pairs of instants of time and then the correlator K_4 is defined.

A2 says that a measurement Q_i do not influence the subsequent dynamics of the system, i.e. the future outcomes q_j are independent from previous observations. With this $p(q_j|Q_i, Q_j, \epsilon) = p(q_j|Q_j, \epsilon)$. By A3, previous measurements do not influence the outcomes of the future ones, meaning that q_i is independent from Q_j. So, equation (4.28) can be rewritten as

$$p(q_i, q_j|Q_i, Q_j, \epsilon) = p(q_i|Q_i, \epsilon)p(q_j|Q_j, \epsilon). \tag{4.30}$$

The authors define the two time correlation functions as

$$C_{ij} = \langle Q_i Q_j \rangle = \int_{q_i}\int_{q_j} dq_i\, dq_j\; q_i q_j\; p(q_i, q_j|Q_i, Q_j). \tag{4.31}$$

With the joint probability in (4.30), the correlation functions become

$$C_{ij} = \int_{\epsilon} d\epsilon\; p(\epsilon)\; \langle Q_i \rangle_\epsilon \langle Q_j \rangle_\epsilon, \tag{4.32}$$

where $p(\epsilon)$ is the probability distribution of the hidden variable ϵ. In the case where four measurements are made at different instants of time ($t_1 < t_2 < t_3 < t_4$), a fourth-order correlator K_4 is obtained. This correlator is defined similarly to the one in the CHSH case for dichotomic observables

$$K_4 = C_{12} + C_{23} + C_{34} - C_{14} < 2. \tag{4.33}$$

This is called the Leggett-Garg inequality of the fourth order, and has the same limit as the CHSH inequality and the same violation limit of $K_4 = 2\sqrt{2}$.

4.4.1 Leggett-Garg Inequalities Violations for a Qubit

In the original work, Leggett and Garg define the two time correlation functions as the expectation value of the product of the operators in the Heisenberg picture in different instants of times

$$C_{ij} = \langle Q_i Q_j \rangle, \tag{4.34}$$

but the operator $Q_i Q_j$ will be Hermitian only when

$$Q_i Q_j = (Q_i Q_j)^\dagger = Q_j^\dagger Q_i^\dagger. \tag{4.35}$$

Given that Q_i and Q_j are Hermitian

$$Q_i Q_j = Q_j Q_i \to [Q_i, Q_j] = 0, \tag{4.36}$$

which means that there are cases where the correlation function will be complex. Because of this, Fritz [75] made the following proposition:

- **Proposition**: While a spatial correlator is given by the expectation value of the tensor product of the observables, a temporal correlator is given by half the expectation value of the anticommutator of the observables:

$$spatial: \; C_{AB} = \langle A \otimes B \rangle \; \to \; temporal: \; C_{ij} = \frac{1}{2}\langle \{Q_i, Q_j\} \rangle, \tag{4.37}$$

which is always real. Now, consider a time evolution of a qubit such that the operators in the Heisenberg picture are given by

$$\sigma_i = \sigma^H(\tau_i) = \hat{m}_i \cdot \vec{\sigma}, \tag{4.38}$$

where the time evolution is encoded in the vector $\hat{m}_i$. Applying these operators in (4.37), we have

$$C_{ij} = \frac{1}{2}\mathrm{Tr}[(\hat{m}_i \cdot \vec{\sigma})(\hat{m}_j \cdot \vec{\sigma})\rho + (\hat{m}_j \cdot \vec{\sigma})(\hat{m}_i \cdot \vec{\sigma})\rho]. \tag{4.39}$$

Remembering that

$$(\hat{m}_i \cdot \vec{\sigma})(\hat{m}_j \cdot \vec{\sigma}) = (\hat{m}_i \cdot \hat{m}_j)\mathbb{1} + i(\hat{m}_i \times \hat{m}_j)\vec{\sigma}, \tag{4.40}$$

then

$$C_{ij} = \frac{1}{2}\mathrm{Tr}[2(\hat{m}_i \cdot \hat{m}_j)\rho] = (\hat{m}_i \cdot \hat{m}_j)\mathrm{Tr}[\rho] = \hat{m}_i \cdot \hat{m}_j, \tag{4.41}$$

which is independent of the initial state. In the case of a spin precessing, the time evolution will be governed by the Hamiltonian $H = \frac{1}{2}\omega\sigma_{\hat{h}}$, where the subscript $\hat{h}$ define the direction of the external homogeneous field. In this case, the vector $\hat{m}_i$ is

$$\hat{m}_i = \cos\tau_i \; \hat{n} + \sin\tau_i \; (\hat{n} \times \hat{h}) + [1 - \cos\tau_i] \; (\hat{n} \cdot \hat{h}), \tag{4.42}$$

where $\hat{n}$ is the direction in which the spin is observed and $\tau_i = \omega t_i$ is the normalized time. Substituting (4.42) in (4.41), the correlation function become

$$C_{ij} = \cos\tau_i \cos\tau_j + \sin\tau_i \ \sin\tau_j \ (\hat{n} \times \hat{h})^2 + (1 - \cos\tau_i \ \cos\tau_j) \ (\hat{n} \cdot \hat{h})^2. \tag{4.43}$$

When $\hat{n} \| \hat{h}$, the correlation functions will be $C_{ij} = 1$ and the correlator of the third order $K_3 = 1$, which do not violate the inequality. This is expected since the spin do not evolve in time and we will make sequential observations of the same spin component in every instant, which are always independent. In the case where $\hat{n} \perp \hat{h}$, the correlation function is $C_{ij} = \cos(\tau_j - \tau_j)$, and the correlator becomes

$$K_3 = \cos(\tau_1 - \tau_2) + \cos(\tau_2 - \tau_3) - \cos(\tau_1 - \tau_3). \tag{4.44}$$

For simplicity, the differences between sequential times can be defined as a fundamental period $\tau_0 = \tau_{i+1} - \tau_i$, such that the correlator is given by

$$K_3 = 2\cos(\tau_0) - \cos(2\tau_0), \tag{4.45}$$

which is maximized at $K_3 = 3/2$ when $\tau_0 = \pi/3 + 2n\pi$ for $n = 0, 1, 2, \ldots$.

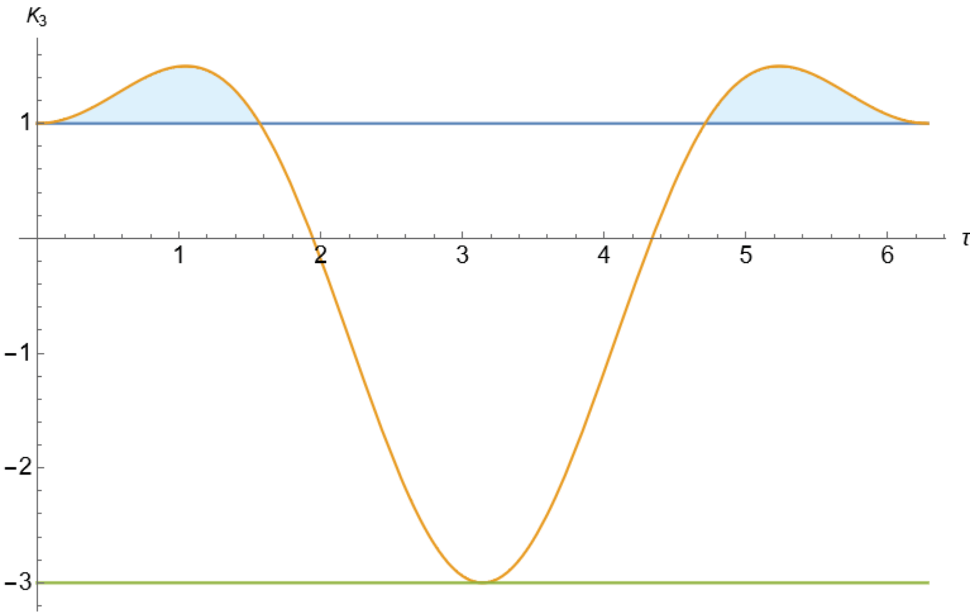


Figure 11 – The correlator K_3 as a function of the period τ_0. The blue line represents the upper bound of the correlator, the green line the lower bound and the shadowed area are the cases when the LGI is violated.

The plot of the correlator (4.45) as a function of τ_0 is given in Figure 11. The shadowed represents the cases where the correlator is violated, the blue line is the upper bound and the green line is the lower bound. The periods where the correlator is violated are $\tau_0 \in (0, \pi/2)$ and $\tau_0 \in (3\pi/2, 2\pi)$.

Before we finish this section, it is interesting to compare the LGIs with the commutation relation of the observables in the Heisenberg picture. Using the relation in (2.76) for $\hat{a} = \hat{m}_i$ and $\hat{b} = \hat{m}_j$, the norm of the commutator becomes

$$||[\hat{m}_i \cdot \vec{\sigma}, \hat{m}_j \cdot \vec{\sigma}]||^2 = 8 - 8(\hat{m}_i \cdot \hat{m}_j)^2 \tag{4.46}$$

or

$$C_{ij} = \left(1 - \frac{||[\sigma_i, \sigma_j]||^2}{8}\right)^{1/2}, \tag{4.47}$$

where $\hat{m}_i \cdot \vec{\sigma} = \sigma_i$ and $\hat{m}_j \cdot \vec{\sigma} = \sigma_j$. Substituting the correlation functions (4.47) in the correlator K_3, we have

$$K_3 = \left(1 - \frac{||[\sigma_1, \sigma_2]||^2}{8}\right)^{1/2} + \left(1 - \frac{||[\sigma_2, \sigma_3]||^2}{8}\right)^{1/2} - \left(1 - \frac{||[\sigma_1, \sigma_3]||^2}{8}\right)^{1/2}. \tag{4.48}$$

This result shows that the LGIs are directly associated with the norm of the commutator, meaning that the LGIs are functions that measures the incompatibility of the spin operators in the Heisenberg picture. This also answer why the correlation functions do not depend on the initial state, differently from the correlator S in the CHSH scenario, which is inherently dependent on the initial state.

4.5 Multi-Irrealism

In this section, inspired by the joint irrealism of CA, we will propose the multi-irrealism for three observables and also introduce the notion of multi-irreality for different temporal phases. After this, we will make a direct comparison with a correlator quantifier inspired by the correlator K_3 and discuss the similarities between them.

For three different observables $A = \sum_n a_n \Lambda_{a_n}$, $B = \sum_m b_m \Lambda_{b_n}$ and $C = \sum_l c_l \Lambda_{c_l}$, we can make a triple sequential map for the state ρ in the similar way it was done for the joint irreality. In this case, the map becomes

$$\Phi_{ABC}(\rho) = \sum_{nml} \Lambda_{c_l} \Lambda_{b_m} \Lambda_{a_n} \rho \Lambda_{a_n} \Lambda_{b_m} \Lambda_{c_l}. \tag{4.49}$$

In direct analogy to the CA joint irrealism, we define that the triple $\{A, B, C\}$ have multi-reality if

$$\Phi_{ABC}(\rho) = \Phi_{CAB}(\rho) = \Phi_{BCA}(\rho) = \Phi_{ACB}(\rho) = \Phi_{BAC}(\rho) = \Phi_{CBA}(\rho) = \rho. \tag{4.50}$$

When this condition is satisfied, the observables are said to be multi-elements of reality for the state ρ. Having that $\Phi_A(\Phi_A(\rho)) = \Phi_A(\rho)$, when (4.50) is true, we can see that $\Phi_A \circ \Phi_A(\Phi_{BC}(\rho)) = \Phi_A(\rho) \rightarrow \Phi_{ABC}(\rho) = \Phi_A(\rho)$, but $\Phi_{ABC}(\rho) = \rho$ so $\Phi_A(\rho) = \rho$. This process can be reproduced for the other two observables B and C. This means that if A, B and C represents joint elements of reality, then they also represents elements of reality individually in BA sense.

Similarly to CA, we define the multi-irreality as

$$\mathfrak{I}_{ABC}(\rho) = \sum_{\substack{i,j,k \\ i\neq j\neq k}} \frac{S(\Phi_{ijk}(\rho))}{6} - S(\rho) \quad ; \; i,j,k = \{A,B,C\}. \tag{4.51}$$

which is always non-negative. Rewriting the multi-irreality by adding and subtracting the entropy of the maps $S(\Phi_A(\rho))$, $S(\Phi_B(\rho))$ and $S(\Phi_C(\rho))$, the multi-irreality can be rewritten in the form

$$\mathfrak{I}_{ABC} = \frac{1}{3}[\mathfrak{I}_{AB}(\Phi_C(\rho)) + \mathfrak{I}_{BC}(\Phi_A(\rho)) + \mathfrak{I}_{AC}(\Phi_B(\rho)) + \mathfrak{I}_A(\rho) + \mathfrak{I}_B(\rho) + \mathfrak{I}_C(\rho)]. \tag{4.52}$$

With the identity

$$\mathfrak{I}_{AB}(\rho) = \frac{\mathfrak{I}_A(\rho) + \mathfrak{I}_B(\rho) + \mathfrak{I}_A(\Phi_B(\rho)) + \mathfrak{I}_B(\Phi_A(\rho))}{2}, \tag{4.53}$$

we can rewrite the first three terms of (4.52) as

$$\mathfrak{I}_{AB}(\Phi_C(\rho)) = \frac{\mathfrak{I}_A(\Phi_C(\rho)) + \mathfrak{I}_B(\Phi_C(\rho)) + \mathfrak{I}_A(\Phi_{BC}(\rho)) + \mathfrak{I}_B(\Phi_{AC}(\rho))}{2}, \tag{4.54}$$

$$\mathfrak{I}_{BC}(\Phi_A(\rho)) = \frac{\mathfrak{I}_B(\Phi_A(\rho)) + \mathfrak{I}_C(\Phi_A(\rho)) + \mathfrak{I}_B(\Phi_{CA}(\rho)) + \mathfrak{I}_C(\Phi_{BA}(\rho))}{2}, \tag{4.55}$$

$$\mathfrak{I}_{AC}(\Phi_B(\rho)) = \frac{\mathfrak{I}_A(\Phi_B(\rho)) + \mathfrak{I}_C(\Phi_B(\rho)) + \mathfrak{I}_A(\Phi_{CB}(\rho)) + \mathfrak{I}_C(\Phi_{AB}(\rho))}{2}. \tag{4.56}$$

Substituting the relation above in (4.52), we have

$$\mathfrak{I}_{ABC}(\rho) = \frac{1}{6}\left[2\mathfrak{I}_A(\rho) + 2\mathfrak{I}_B(\rho) + 2\mathfrak{I}_C(\rho) + \sum_{\substack{i,j \\ i\neq j}} \mathfrak{I}_i(\Phi_j(\rho)) + \sum_{\substack{i,j,k \\ i\neq j\neq k}} \mathfrak{I}_i(\Phi_{jk}(\rho))\right]. \tag{4.57}$$

Since the BA irreality can be written as the relative entropies, we know that they are non-negative and goes to zero only if the maps are equal to the state. As a consequence of this, the multi-irreality is zero if $\rho = \Phi_i(\rho) = \Phi_{ij}(\rho) = \Phi_{ijk}(\rho)$, for $i,j,k = \{A,B,C\}$, which corresponds to the definition of multi-irrealism in (4.50). Not only that, but this shows that when the triple A, B, C have multi-reality, then the pairs will have joint-reality and they will also have individual elements of reality, showing that the definition of multi-irrealism is capable to supplement the definitions CA joint irrealism and BA irrealism.

Now, we will propose that, instead of using three different observables, we may apply the multi irreality to the same physical quantity in three different instants of time, such as A_1, A_2 and A_3, given that $A_i = A^H(t_i)$. At first, this may sound an absurd, since there will be cases where the sequential map will be constructed in a sequence where the non-revealed measurement is made in future times before the previous one, such as $\Phi_{A_1A_2A_3}(\rho)$. But, this can be resolved by defining the instant of time as a parameter of some unitary transformation.

As an example, let us use the time evolution of the spin precessing dynamics. This operator in $t_1 = 0$ is $\sigma_1 = \hat{n} \cdot \vec{\sigma}$ and for a time $t_2 = \pi/2$ the spin will be $\sigma_2 = [(\hat{n} \times \hat{h}) + (\hat{h} \cdot \hat{n})\hat{h}] \cdot \vec{\sigma}$. In this case, we can see that time do not play the role of defining a sequence of events, but it is just a parameter that represents some configuration for the operator, in a way that we can make a observation of $\vec{\sigma}_2$ and then $\vec{\sigma}_1$.

Now we are ready to define the multi-irreality in time. For an observable in the Heisenberg picture, such as $A_i = A^H(t_i) = \sum_n a_n \Lambda_{a_n}(t_i)$, the observable A will satisfy multi-ireality in time if

$$\Phi_{123}(\rho) = \Phi_{312}(\rho) = \Phi_{231}(\rho) = \Phi_{132}(\rho) = \Phi_{213}(\rho) = \Phi_{321}(\rho) = \rho. \tag{4.58}$$

With this, we extend the multi-irreality to different temporal phases as

$$\mathfrak{I}_{123}(\rho) = \sum_{\substack{i,j,k=1 \\ i\neq j\neq k}}^{3} \frac{S(\Phi_{ijk}(\rho))}{6} - S(\rho), \tag{4.59}$$

which is zero if and only if the condition (4.58) is satisfied.

Our objective now is to compare the multi-irreality in time with the correlator of Leggett-Garg and see if they share some aspects or if they are correlated. As an example, we will apply both in the spin precessing dynamics.

To determine the multi-irreality, we will use the simplified irreality for a spin system. Suppose we have a generic state $\rho_{\vec{r}} = \frac{\mathbb{1} \pm \vec{r}\cdot\vec{\sigma}}{2}$, with eigenvalues $\lambda_\pm = \frac{1 \pm r}{2}$. We can see that $\lambda_+ = 1 - \lambda_-$, and therefore we can determine the entropy of the state $\rho_{\vec{r}}$ by the quantum binary entropy. The state after a non-revealed measurement $\Phi_{\sigma_{\hat{n}}}$ in a general direction $\hat{n}$ is given by

$$\Phi_{\sigma_{\hat{n}}}(\rho_{\vec{r}}) = \frac{\mathbb{1} + (\hat{n} \cdot \vec{r})\hat{n} \cdot \vec{\sigma}}{2}, \tag{4.60}$$

with eigenvalues $\lambda_\pm = \frac{1}{2}(1 \pm |\hat{n} \cdot \vec{r}|)$. The entropy of the map can also be computed with the binary quantum entropy. In the case of the multi-irreality, the sequential map for the spin precessing $\hat{m}_i \cdot \vec{\sigma}$ in three different instants of time t_i, t_j and t_k is

$$\Phi_{ijk} = \frac{\mathbb{1} + (\hat{m}_i \cdot \vec{r})(\hat{m}_i \cdot \hat{m}_j)(\hat{m}_j \cdot \hat{m}_k)\hat{m}_k \cdot \vec{\sigma}}{2}, \tag{4.61}$$

with eigenvalues

$$\lambda_{ijk,\pm} = \frac{1 \pm |(\hat{m}_i \cdot \vec{r})(\hat{m}_i \cdot \hat{m}_j)(\hat{m}_j \cdot \hat{m}_k)|}{2}. \tag{4.62}$$

It is interesting to notice that the positive eigenvalues of the maps depend on the absolute value of the two time correlation functions that we have in the LGIs ($C_{ij} = \hat{m}_i \cdot \hat{m}_j$), and the multi-irreality $\mathfrak{I}_{123}$ will have a dependence of the correlation functions C_{ij}. Indeed, the entropy of the map Φ_{ijk} is given by

$$S(\Phi_{ijk}) = -\lambda_{ijk,+}\log_2\lambda_{ijk,+} - (1-\lambda_{ijk,+})\log_2(1-\lambda_{ijk,+}), \tag{4.63}$$

where we use the *bit* scale of information. Substituting (4.62) in (4.63)

$$\begin{aligned} S(\Phi_{ijk}) = &-\left(\frac{1+|(\hat{m}_i\cdot\vec{r})C_{ij}C_{jk}|}{2}\right)\log_2\left(\frac{1+|(\hat{m}_i\cdot\vec{r})C_{ij}C_{jk}|}{2}\right) \\ &-\left(1-\frac{1+|(\hat{m}_i\cdot\vec{r})C_{ij}C_{jk}|}{2}\right)\log_2\left(1-\frac{1+|(\hat{m}_i\cdot\vec{r})C_{ij}C_{jk}|}{2}\right). \end{aligned} \tag{4.64}$$

And the entropy of the state $\rho_{\vec{r}}$ is

$$\begin{aligned} S(\rho_{\vec{r}}) = &-\left(\frac{1+|\hat{n}\cdot\vec{r}|}{2}\right)\log_2\left(\frac{1+|\hat{n}\cdot\vec{r}|}{2}\right) \\ &-\left(1-\frac{1+|\hat{n}\cdot\vec{r}|}{2}\right)\log_2\left(1-\frac{1+|\hat{n}\cdot\vec{r}|}{2}\right). \end{aligned} \tag{4.65}$$

So, using the relations (4.64) and (4.65), we are able to compute the multi-irreality $\mathfrak{I}_{123}$.

The direct comparison between the multi-irreality and the LGIs correlator can be problematic, since the correlator K_3 does not share the same domain as the multi-irreality. The correlator has values $-3 \leq K_3 \leq 1$ when the system is macrorealistic and $1 < K_3 \leq 3/2$ when the system is not macrorealistic. However, we can manipulate the domain of the violated correlator in such a way that it will have the same range as the multi-irreality. Given that

$$1 < K_3 \leq 3/2, \tag{4.66}$$

then

$$0 < 2(K_3 - 1) \leq 1. \tag{4.67}$$

To discard the negative values, we define the correlator quantifier $K_3' = \max[0, 2(K_3-1)]$. When $K_3' > 0$, the system is not macrorealistic and when $K_3' = 0$, the system is macrorealistic.

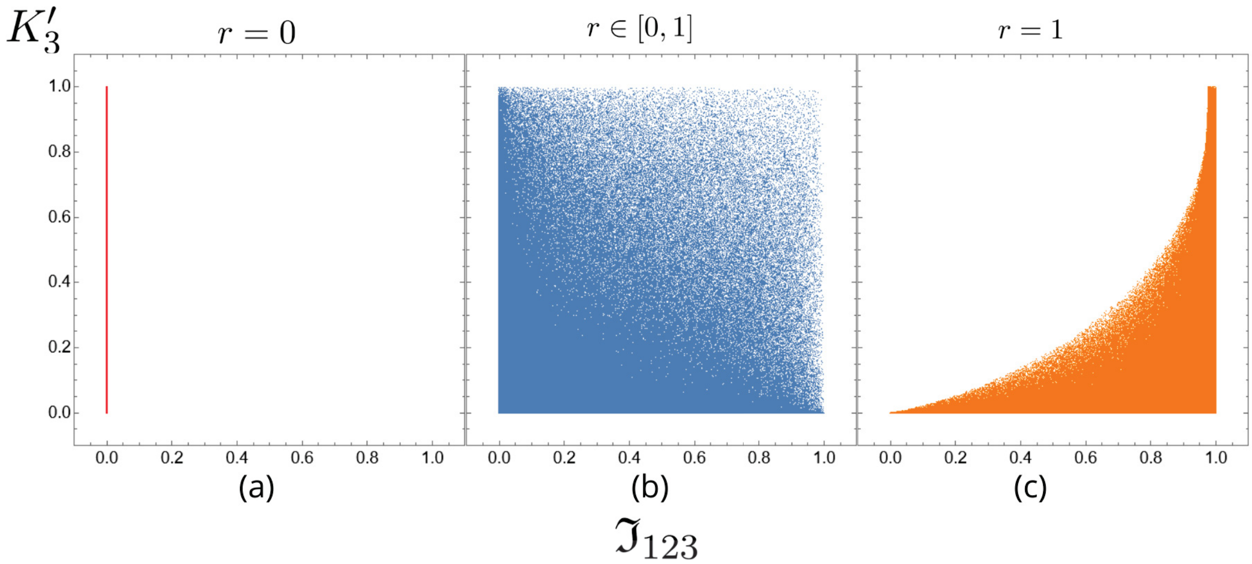


Figure 12 – Compassion between $\mathfrak{I}_{123}$ and K_3' for 10^6 values of the components of $\hat{n}(\theta_n, \phi_n)$, $\hat{h}(\theta_h, \phi_h)$, $\rho_{\vec{r}}(\theta_r, \phi_r, r)$ and the instants of time t_1, t_2, t_3. (a) is for maximally mixed states, (b) is for mixed states and (c) is for pure states.

In Figure 12, we compare K_3' with $\mathfrak{I}_{123}$ for 10^6 values of the components of the external magnetic field $\hat{h}(\phi_r, \theta_r)$, the components of the observed spin $\hat{n}(\phi_n, \theta_n)$, the components of the state $\rho_{\vec{r}}(\phi_r, \theta_r, r)$ and the instants of time t_1, t_2 and t_3 for $t_1 < t_2 < t_3$.

For maximally mixed states (Figure 12 (a)), multi-irreality is always zero, as expected since the sequential maps do not change the state, and the correlator admits all possible values. For mixed states (Figure 12 (b)), we see a reduction of the densities of the dots when both the quantities comes to 1, but this could be caused by the way the values were chosen. For pure states (Figure 12 (c)), we see that the quantities are are limited, in a way that $\mathfrak{I}_{123} \geq K_3'$ and the equality holds in the extremes 1 and 0. This shows that the violation of macrorealism is sufficient for multi-irrealism, but not necessary. Indeed, we can see that when there is no violation of macrorealism ($K_3' = 0$), the multi-irrealism is possible ($\mathfrak{I}_{123} > 0$). This is expected, since when the assumption A2 is violated, violating macrorealism, multi-irrealism can occur, since the measurement was invasive and could disturb the state of the system.

CHAPTER 5

Conclusions

Time is one of the most fundamental concepts in physics, yet it remains incompletely understood. The objective of this work is to advance the understanding of time in quantum mechanics. To achieve this, we explore the properties and applications of time observables, as well as investigate the temporal correlations that arise in dynamical systems.

Initially, we reviewed the three possible types of time in physical theories: external, intrinsic, and observable. The second type, intrinsic time, exhibits direct properties in quantum theory, redefining the concept of the time-energy uncertainty relation. In the section on observable time, we addressed the challenge of defining a time operator due to Pauli's objection and presented two approaches from the literature to circumvent this issue: first, through a non-self-adjoint time operator, and second, by using an external clock entangled with the system. In the same chapter, we revisited the complementarity principle and demonstrated that creating which-way information requires entangling the spatial modes of an interferometer with a degree of freedom of the system.

In the final section of Chapter 3, we explored an interesting application of the time observable in interferometers. We concluded that if time is indeed an observable in quantum mechanics, then the ket states corresponding to different times of flight should be capable of becoming entangled with their respective spatial modes in interferometers. This entanglement would create which-way information, thereby destroying interference patterns. Then, we examined the Fizeau interferometer and argued that, if the time of flight generates which-way information, this interferometer represents a promising candidate for observing such a phenomenon.

However, we also discussed that the theoretical description of this phenomenon poses significant challenges. Specifically, the theory does not provide a clear framework for measuring the dispersion of the time observable, which hinders further theoretical exploration. In future work, we aim to apply this concept to matter-wave interferometers, with the goal of employing different approaches to analyze the dispersion of time observables and determine the scale at which time should exhibit its quantum behavior.

In the second part of our work, we conducted an extensive review of locality and determinism in quantum mechanics, focusing on Bell's theorem, the CHSH inequality, the irrealism of BA, and Leggett-Garg macrorealism. An interesting result we obtained in this section is that, for spin systems, the two-time correlation functions in the LGIs are directly related to the norm of the commutator of the same spin operator in the Heisenberg picture at two different instants of time. This implies that the LGIs essentially serve as a function quantifying the degree of incompatibility between Heisenberg operators at different times. Furthermore, this relationship explains why the LGIs, unlike the CHSH inequality, do not depend on the initial state of the system.

In the final part of our work, we extended the definition of joint irrealism to three physical quantities and introduced a new quantifier, which we termed multi-irreality. This quantifier determines whether three observables represent multi-elements of reality for a given system. We demonstrated that this new quantity complements previous definitions, showing that if three observables represent multi-elements of reality, then their pairs also represent CA joint elements of reality, as well as BA elements of reality individually. In future work, we aim to further explore this concept by investigating potential implementations of multi-irreality and identifying relevant case studies. Additionally, we plan to generalize this framework to n observables and examine its broader implications

In the same section, we extended the definition of multi-irreality to dynamical observables and conducted a direct comparison with a correlator quantifier for the Leggett-Garg inequalities. We observed certain tendencies, particularly in the case of a pure state, where a violation of macrorealism is sufficient for multi-irrealism but not necessary. In future works, we aim to deepen our understanding of the relationship between these two quantities by investigating the correlation between them. Additionally, we plan to study the states and systems that give rise to the frontier observed in the case of pure states.

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