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Characterization and applications of quantum measurement invasiveness

Caractérisation et applications de l'invasivité de la mesure quantique

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Jury

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Abstract

Quantum measurement invasiveness is a feature of quantum phenomena, *i.e.* associated with the fact that measurements can affect quantum systems in a manner which cannot be described by classical physics. In this thesis, we will investigate measurement invasiveness through the Leggett-Garg inequality and another inequality based on the *non-disturbance condition*, both of which, when violated, witness measurement invasiveness.

First, we will study a model for the violation of the Leggett-Garg inequality, which will allow us to provide an operational characterization of measurement invasiveness through a parameter called the *measurability* of the physical system. This parameter controls Leggett-Garg inequality violation and can be associated with experimental tests of this inequality, helping one to understand and interpret them. We will also investigate, through this model, the relationship between measurement invasiveness and a specific definition of macroscopicity, related to the “size” of spin systems.

We will then seek to study an application of measurement invasiveness in the context of protocols for parameter estimation or *quantum metrology*. A general relationship between the Fisher information and temporal quantum correlations will be established, allowing one to characterize the robustness of metrological scenarios against the presence of noise. This relationship will also serve as a guideline for a connection between measurement invasiveness and (nearly-)optimal metrological scenarios. We will also establish a relationship between measurement invasiveness and a definition of a measure of macroscopic coherence.

Lastly, we will propose a protocol for testing measurement noninvasiveness based on the non-disturbance condition for spin systems of arbitrary size. This inequality allows one to argue against the possibility of its violation being due to the classical disturbance of measurements. We will show that the maximum value for the violation of this inequality corresponds to the number of particles which constitutes the system.

Keywords: quantum measurement; measurement invasiveness; Leggett-Garg inequality; quantum metrology; rmacroscopic realism.

Résumé

L'invasivité de la mesure quantique est une propriété des phénomènes quantiques. Elle est reliée au fait que la mesure de systèmes quantiques peut les affecter d'une façon que ne peut pas être décrite au sein de la physique classique. Cette thèse tudie la question de l'invasivité des mesures quantiques à travers l'inégalité de Leggett-Garg et d'une autre inégalité basée sur la condition de non perturbation (" non-disturbance condition "). La violation de ces inégalités témoignent de l'invasivité des mesures quantiques.

Dans un premier temps, nous étudierons un modèle pour la violation de l'inégalité de Leggett-Garg, qui permettra une caractérisation opérationnelle de l'invasivité de la measure quantique à travers un paramétre appelé la mesurabilité du système physique. Ce paramètre contrôle la violation de l'inégalité de Leggett-Garg et peut être reliée à des tests expérimentaux de cette ingalité. De cette façon, ce paramétre permet la comprehénsion et l'interprétation de ces violations. Nous avons également étudié, via ce modèle, la relation entre l'invasivité et une définition particuliére de la " macroscopicité ", associée la " taille " de systèmes de spin.

Nous avons ensuite étudié une application de l'invasivité de la measure quantique dans le cadre des protocoles pour l'estimation de param´etres en métrologie quantique. Une relation générale entre l'information de Fisher et les corrélations quantiques temporelles a été établie, et permet la caractérisation de la robustesse au bruit de scenarios de métrologie. Cette relation sert de ligne directrice pour la connexion entre l'invasivité de la mesure quantique et des scenarios (quasi-)optimaux en métrologie. Nous avons également établi une relation entre l'invasivité de la mesure quantique et une définition de la cohérence macroscopique.

Pour finir, nous avons proposé un protocole pour tester la non-invasivité de mesures, basé sur la condition de non perturbation, pour des systèmes de spin de taille arbitraire. Cette inégalité permet de s'assurer contre la possibilité que sa violation soit due á des perturbations classiques de la mesure. Nous avons montré que la valeur maximale pour la violation de l'inégalité correspond au nombre de particules qui constitue le systéme.

Mots clefs : mesure quantique; invasivité de la mesure; inégalité de Leggett-Garg; métrologie quantique; réalisme macroscopique.

Résumé substantiel

La théorie quantique est certainement une des théories scientifiques les plus révolutionnaires elaborées au début du 20ème siècle et developpées depuis. Le formalisme quantique a été concevé dû à l'incapacité de la théorie classique de décrire les résultats de quelques expériences realisées avec des systèmes *microscopiques*, comme des atomes ou des photons, où le terme "microscopique" est defini par rapport à un certain paramètre du système, e.g. la masse, la taille etc. De cette façon, la théorie quantique entraine plusieurs défis à notre intuition, la dernière étant basée sur la physique classique. Comme a bien été remarqué par Leggett [Leggett, 2002],

> Quantum mechanics is very much more than just a 'theory'; it is a completely new way of looking at the world [...]

Ainsi, les phénomènes *non-classiques* décrits par la théorie quantique se retrouvent au-delà de la capacité descriptive et prédictive de la physique classique. Dans le chapitre 2, nous discutons certains d'entre ces phénomènes non-classiques dans le cadre d'une concise présentation générale de la théorie quantique, phénomènes comme l'interference quantique, liée au concept non-classique de la *superposition* d'états, et la non-localité, lié au concept de l'*intrication.* Nous y discutons également un autre concept important pour cette thèse, relié à la nature non-deterministe de la théorie quantique, c'est-à-dire le concept de la mesure de systèmes quantiques. Le terme "non-deterministe" est associé au fait que les résultats de la mesure de systèmes quantiques ne peuvent pas être *toujours* prévus avec certitude. La mesure de systèmes quantiques constitue, par conséquence, encore un de ses aspects qui ne peuvent pas être décrits selon les lois de la physique classique. De façon générale, le problème lié à l'interpretation de la mesure en physique quantique est appelé le *problème de la mesure* [Leggett, 2005].

Malgré le fait que la théorie quantique a été originalement formulée en réponse aux écarts des résultats de quelques expériénces dans le cadre de systèmes microscopiques par rapport à la description classique, il est naturel de se demander si ces phénomènes non-classiques pourraient être observés à une échelle macroscopique, définie par rapport à un paramètre donné [Leggett, 2002, Arndt and Hornberger, 2014, Knee et al., 2016, Formaggio et al., 2016, Ghirardi et al., 1986]. Cette question fondamentale

de la validité de la théorie quantique à l'échelle macroscopique a déjà été formulée en 1935 par Schrödinger [Schrödinger, 1935].

Dans ce manuscrit, nous nous concentrons sur la notion non-classique de l'*invasivité de la mesure*, liée au fait que la mesure peut affecter l'évolution de systèmes quantiques d'une façon qui ne peut pas être décrite par la théorie classique. Plus spécifiquement, la notion de l'invasivité de la mesure est définie comme l'impossibilité d'obtenir, à partir de la distribution de probabilité globale du résultat de deux mesures séquentielles de systèmes quantiques et à travers le marginal de cette probabilité globale sur les résultats de la première mesure, le résultat de la deuxième mesure individuellement. Dans le but d'étudier l'invasivité de la mesure, nous emploierons principalement l'*inégalité de Leggett-Garg*, qui est définie par la somme de correlations entre les résultats de deux mesures effectuées sur un système physique qui évolue dans le temps, sa violation étant un témoin de l'invasivité de la mesure. Nous présenterons également ces concepts dans le chapitre 2, où nous établirons d'abord le cadre pour cette présentation à travers l'introduction du formalisme général pour la *contextualité* de la théorie quantique.

Dans le chapitre 3, nous introduisons un modèle opérationnel pour la violation de l'inégalité de Leggett-Garg, où les effets de l'invasivité de la mesure sont controlables à travers un paramètre associé à la definition de *mesurabilité* du système physique. Ce paramètre est lié à des measures generalisées, et qui peuvent être associées à la dimension du système, erreurs de mesure, ou *back action*. Ce modèle permet, par conséquence, l'étude de la relation entre l'invasivité de la mesure et une definition spécifique de la macroscopicité de systèmes de spin-j, caractérisée par la magnitude de j, la "taille" du spin.

Ensuite, dans le chapitre 4, nous étudierons une application pour le concept de l'invasivité de la mesure dans le cadre de protocoles pour l'estimation de paramètres. Le cadre général de cette théorie, pour des systèmes classiques aussi bien que quantiques, est introduit dans le chapitre 2. La théorie de l'estimation de paramètres est l'objet d'étude de la métrologie quantique, qui a pour but l'emploi de systèmes quantiques afin de surpasser la précision possible en utilisant des systèmes classiques. Nous investiguerons la connexion entre l'inégalité de Leggett-Garg et des scénarios optimales du point de vue de la métrologie quantique, et cette connexion nous permettra d'associer scénarios (quasi-)optimales en métrologie avec des scenarios où l'inégalité de Leggett-Garg est violée. Ainsi, une connexion entre l'invasivité de la mesure et des scénarios en métrologie plus ou moins favorables est établie. Comme dans le chapitre 2, nous illustrons les résultats en utilisant un modèle pour des systèmes de spin.

Finalement, dans le chapitre 5, nous explorons une inégalité basée sur la *condition de non-perturbation*. Cette inégalité est une alternative à l'inégalité de Leggett-Garg, sa violation étant aussi un témoin de l'invasivité de la mesure, et qui permet que l'on argumente contre la possibilité d'expliquer cette violation comme résultat de perturbations classiques au lieu d'un effet non-classique. Nous proposons un protocole qui permet de tester l'invasivité de la mesure pour des systèmes de spin-j de dimension arbitraire, pour lesquels la valeur maximale de la violation de l'inégalité correspond au nombre de particules du système.

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Contents

Chapter 1

Introduction

Quantum theory is certainly one of the most revolutionary theories devised in the beginning of the 20th century and developed from then on. Quantum formalism was formerly conceived in view of the failure of classical physics to describe the results of experiments involving *microscopic* systems such as atoms and photons, where the term "microscopic" is defined in relation to a given parameter of the system, such as mass, size etc. In this way, the advent of quantum theory brought about numerous challenges to our classical-physics-based intuition. As pointed out by Leggett [Leggett, 2002],

> Quantum mechanics is very much more than just a 'theory'; it is a completely new way of looking at the world [...]

Indeed, the *nonclassical* phenomena described by quantum theory are beyond the scope of the predictions and descriptive capacity of classical physics. In chapter 2, we will discuss some of these nonclassical phenomena by providing a brief overview of quantum theory, phenomena such as quantum interference, related to the nonclassical notion of *superposition* of states, and nonlocality, associated with the concept of *entanglement*. Another important element for this thesis, related to the non-deterministic nature of quantum theory, is the concept of measurement of quantum systems. The term "non-deterministic" is related to the fact the results of measurements of quantum systems cannot be predicted with certainty. Quantum measurements are, therefore, another feature of quantum theory characterized by a strikingly departure from the classical description. Issues concerning the different interpretations of quantum measurements in quantum theory are, in general, referred to as the *quantum measurement problem* [Leggett, 2005].

Despite the fact that quantum physics was originally formulated in response to the deviations of the results of experiments performed at a microscopic level, it is natural to ask the question of whether such nonclassical phenomena could also be observed at a *macroscopic* scale, defined with respect to a given parameter [Leggett, 2002, Arndt and Hornberger, 2014, Knee et al., 2016, Formaggio et al., 2016, Ghirardi et al., 1986]. This fundamental question concerning the validity of extrapolating quantum mechanics to the macroscopic world was formulated as early as 1935 by Schrödinger [Schrödinger, 1935].

In this thesis we will focus on the nonclassical notion of *measurement invasiveness*, which accounts for the fact that measurements can affect the evolution of quantum systems in a manner which cannot be described classically. Specifically, the notion of measurement invasiveness is defined as the impossibility of a joint probability distribution of obtaining the results of two subsequent measurements on a quantum system to describe, by taking the marginals of the joint probability over the results of the first measurement, the result of the second measurement individually. To investigate measurement invasiveness, we will mainly use the *Leggett-Garg inequality*, which consists of a sum of correlations between the results of the two measurements, of which the violation is a witness of measurement invasiveness. We will also present these concepts in chapter 2, by first establishing the context for this presentation by introducing a general framework for the *contextuality* of quantum theory.

In chapter 3, we will introduce an operational model for the violation of the Leggett-Garg inequality where the effects of measurement invasiveness are controllable through a parameter associated with what is defined as the *measurability* of the physical system. This parameter is associated with different generalized measurements that can be associated with the dimensionality of a system, measurement errors, or back action. This model will also permit us to investigate the relationship of measurement invasiveness and a specific definition of the macroscopicity for spin-j systems, characterized by the magnitude of j, the "size" of the spin.

Next, in chapter 4, we will seek to investigate an application for the concept of measurement invasiveness in the context of protocols for parameter estimation. The background for this discussion is presented in chapter 2, where we introduce the general framework of the classical and quantum theory of parameter estimation. The quantum theory of parameter estimation is the object of study of *quantum metrology*, of which goal is to employ quantum systems in order to improve the precision of estimation beyond what is possible by using classical systems. Therefore, we will investigate the connection between the Leggett-Garg inequality and optimal scenarios from the point of view of quantum metrology, and this connection will allows us to associate (nearly-)optimal metrological scenarios to scenarios in which the Leggett-Garg inequality is violated. In this way, a connection between measurement invasiveness and more or less favorable metrological scenarios is established. As well as in chapter 2, we illustrate our results by using a model for spin systems.

Finally, in chapter 5, we will explore an inequality based on the *non-disturbance condition*, which is an alternative to the Leggett-Garg inequality also ruling out measurement noninvasiveness. This inequality allows one to argue against the possibility of explaining its violation as a result of classical disturbance, instead of a nonclassical effect. We will propose a protocol allowing one to witness measurement invasiveness for arbitrary spin-j systems, and show that the maximal value for this violation corresponds to the number of particles of the system.

Chapter 2

Quantum theory: an overview

In this chapter, we give an overview of quantum theory focusing on the ingredients which are fundamental to the comprehension of the following chapters, in an effort to present a self-contained thesis. However, we do not intend to provide a complete review, and some familiarity with quantum theory is required on the part of the reader.

We start by introducing the general framework of quantum theory, which is then followed by the presentation of some other important features for this work, namely contextuality, quantum correlations, and the classical and quantum theory of parameter estimation.

2.1 The general framework of quantum theory

2.1.1 Interference, the evidence for quantum theory

At the core of the conception of quantum theory in the 20th century, were experimental deviations of classical physics' predictions at the level of single atoms, electrons and photons - one can cite as examples the photoelectric effect, the Davisson-Germer experiment and other realizations [Davisson and Germer, 1927, Einstein, 1905, von Halban and Preiswerk, 1936, Estermann and Stern, 1930, Gähler and Zeilinger, 1991]. In order to describe the oddness of quantum systems in relation to our (classical) intuition, we analyze, in the following, a double-slit experiment, also known as *Young experiment*, which has been already used in the context of classical physics to demonstrate the *wave nature* of light through the observation of interference. In the following description, based on Leggett's [Leggett, 2002], the term *microscopic* refers to systems at the atomic or subatomic level, for instance.

Consider the double-slit experiment sketched in Fig. 2.1 performed by using a *quantum system*. This system is constituted of microscopic systems, for instance particles such as electrons, sent by a source S and which will be detected on a screen. It is possible for the particles to take two paths, represented by slits 1 and 2, in order to reach the spot D, where one places a detector. If the slit 1 is closed, one can state with certainty that a particle detected at D went through slit 2 - we will call the associated probability that this happens p_2; correspondingly, if slit 2 is blocked, the probability of detecting the particle at D is p_1, since in that case one knows that it assuredly went through slit 1 before reaching D. On the other hand, if both slits are open, the *total* probability that a particle arrives at D is p_{12}. From our classical intuition, we expect that

$$p_{12} - (p_1 + p_2) = 0. \tag{2.1}$$

However, for quantum systems, whenever there is the possibility of such systems take one or another path out of two paths, it is a well-established experimental fact that [Carnal and Mlynek, 1991, Nairz et al., 2001, Keith et al., 1991, Rauch et al., 1974, Kunze et al., 1997, Rasel et al., 1995, Giltner et al., 1995, Cotter et al., 2015]

$$p_{12} - (p_1 + p_2) = K \neq 0. \tag{2.2}$$

Therefore, within the context of the double-slit experiment with quantum systems, this can be expressed as follows: the total probability p_{12} of detecting a particle at D, which corresponds to a situation in which both slits are opened[1] , is not equal to the sum of p_1 and p_2, the probabilities of detecting at D when one of the slits, 1 or 2, is respectively obstructed. As we will see below, the mathematical description of these results can be done by assigning complex amplitudes c_1 and c_2 to each one of the alternative

[1]Here, we consider that no information about a particle's path, the so-called *which-path information*, is available. For a more general description which considers this possibility, see [Englert, 1996, Wootters and Zurek, 1979, Bagan et al., 2016].

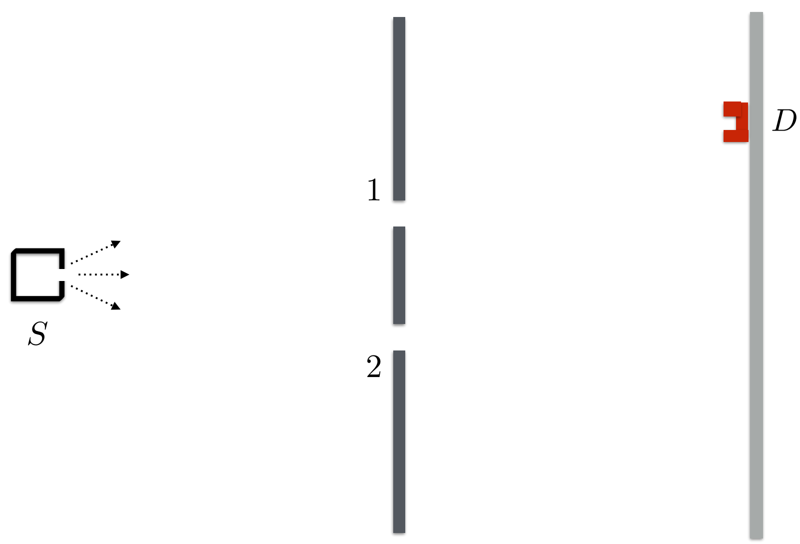

Figure 2.1: Representation of a double slit experiment: a source S emit particles towards the obstacle with slits 1 and 2. A fraction of these particles will be eventually detected by a detector placed on a spot D over a screen.

paths, in such a way that the probabilities are given by

$$
\begin{aligned}
p_1 &= |c_1|^2, \\
p_2 &= |c_2|^2, \\
K &= 2\Re[c_1^* c_2].
\end{aligned}
\tag{2.3}
$$

Thus, it follows that a *quantum-mechanical* description is mathematically identical to the classical description of interference of classical waves in Young's double-slit experiment. By referring to this analogy, K can be named the *interference term*. This term, as pointed out by Leggett, is a experimental *evidence* for quantum theory. The consequence of $K \neq 0$ is that, in an experiment with both slits open, one is not able to assert whether each particle of the ensemble takes its way through either slit 1 or 2.

This conclusion, based on experiments, is clearly in conflict with classical physics. For a system described by classical physics, once one knows the system's initial configuration (e. g. position, momentum), one can in principle predict *deterministically* the system's future configurations from Newtonian laws. As we will present below, the time evolution of the aforementioned amplitudes within the formalism of quantum mechanics is also deterministic. Nevertheless, whether these amplitudes can be associated with entities existing in the real word is a question which is at the core of the different existent interpretations of quantum formalism, which can be classified according to two main positions: *epistemic* and *ontic* [Leifer, 2014]. The first, the epistemic, is the view that quantum theory is not a science which can be directly connected with the real world, but rather a science of information, predictions of which can be confirmed by experiments. The second, the ontic, is the hypothesis that the quantum theory describes the real state of physical systems and therefore has a direct connection with reality.

In this chapter and throughout this thesis, we will present quantum formalism from the perspective of the epistemic view, or, more specifically, from the perspective of the Copenhagen interpretation. However, we will attempt to present some features of quantum formalism independently of any interpretation whenever possible.

2.1.2 Quantum states

In the above described double-slit experiment, there are two mutually exclusive paths which can be taken by the particles, represented by slits 1 and 2. Alternatively, one could also use as example the quantum description of the polarization of light. Polarization is a property of electromagnetic waves, passed on to photons in a quantized description of the field. In this way, by labelling the "up" and "down" polarizations as "1" and "2", this system can be formally described by the general framework which we will introduce in this section.

We then proceed by using the useful and compact notation introduced by Dirac [Dirac, 1939], through which one can associate to these two mutual exclusive alternatives the ortogonal states $|1\rangle$ and $|2\rangle$. Let us consider the *quantum states* of this system which can be mathematically expressed as

$$|\psi\rangle = c_1 |1\rangle + c_2 |2\rangle , \tag{2.4}$$

where c_1 and c_2 are complex amplitudes, $c_1, c_2 \in \mathbb{C}$. In the context of the double-slit experiment described above, $|c_1|, |c_2| \neq 0$ correspond to the situation where the two slits are opened, leading consequently to quantum interference. Whenever this is the case, the quantum state $|\psi\rangle$ is referred to as a *superposition* of the states $|1\rangle$ and $|2\rangle$. The states $|1\rangle$ and $|2\rangle$ are *orthonormal eigenstates*, as they satisfy

$$\langle i \,|\, j\rangle = \delta_{i,j}, \tag{2.5}$$

where $i, j = 1, 2$. The symbol $\langle i|$ is named a *bra*, which is anti-linearly associated with the ket $|i\rangle$, that is $(\lambda\,|i\rangle)^\dagger \rightarrow \lambda^* \langle i|$, λ being a complex number.

Formally, the quantum state of a physical system is characterized by a mathematical object: a state vector in a vector space possessing inner product, the so-called Hilbert space $\mathscr{H}$. A linear *operator* $\mathbf{A}$ defined over $\mathscr{H}$, which is associated with a measurable physical quantity, is called an *observable*. The possible values for the physical quantity that one can measure in the system, as we will see below, correspond to the eigenvalues of the observable $\mathbf{A}$. Hence, an observable must satisfy the condition $\mathbf{A} = \mathbf{A}^\dagger$, in order to have a real *spectrum* $\lambda_1, \lambda_2, ..., \lambda_n$ of eigenvalues, n being therefore the dimension of $\mathscr{H}$. Operators satisfying this condition are called *hermitian operators*. The eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$ are associated with the eigenstates $|1\rangle, |2\rangle, ..., |n\rangle$, respectively, which in turn satisfy the orthonormality condition (2.5) with $i, j = 1, 2, ..., n$ [2].

Using Dirac's notation, $\mathbf{A}$ can therefore be represented in its diagonal form as

$$\mathbf{A} = \sum_i^n \lambda_i \,|i\rangle \langle i|\,, \tag{2.6}$$

where $|i\rangle \langle i|$ represents the diagonal matrix elements of $\mathbf{A}$. A quantum state can then be written in its general form in the *basis* constituted of the eigenstates $|i\rangle$ as

$$|\Psi\rangle = \sum_i^n c_i \,|i\rangle\,, \tag{2.7}$$

with $c_i \in \mathbb{C}$.

[2] This is only valid if the eigenvalues are *non-degenerate*, *i. e.*, if to each eigenvalue λ_i is associated only one eigenstate $|i\rangle$. For a description of a situation in which the spectrum is degenerate, see [Cohen-Tannoudji et al., 1973] or [Sakurai, 1994], for instance.

For a continuous system, considering for instance the position of a particle in one of the directions x, y, z as observable, e. g. by defining the observable $\mathbf{X}$, to which the eigenstates $|x\rangle$ and corresponding eigenvalues x, (2.6) are associated, must be expressed using an integral

$$|\Psi\rangle = \int \psi(x)dx, \tag{2.8}$$

where $\psi(x)$ are complex functions of the position x called *wavefunctions*. Analogously to (2.4), the orthonormality of the eigenstates $|x\rangle$ can in turn be expressed through the following relation:

$$\langle x' \,|\, x'' \rangle = \delta(x' - x''), \tag{2.9}$$

where $\delta(x - x')$ is the Dirac delta function.

By applying a linear transformation $\mathbf{T}$ to the quantum state (2.7), it can be expressed in a different basis of which the eigenstates are $|i'\rangle$ with correspondent complex coefficients c_i':

$$|\Psi'\rangle \equiv \mathbf{T}\,|\Psi\rangle = \sum_{i'}^{n} c_i' \,|i'\rangle\,, \tag{2.10}$$

$\mathbf{T}$ must preserve norm and orthogonality,

$$\mathbf{T}\mathbf{T}^{\dagger} = \mathbb{I}, \tag{2.11}$$

in such a way that $\langle i' \,|\, j' \rangle = \delta_{i'j'}$. Thus, as it preserves orthonormality, $\mathbf{T}$ is called a *unitary* transformation.

2.1.3 Evolution in time of quantum states

A quantum state $|\Psi(t)\rangle$ at time t can be written as

$$|\Psi(t)\rangle \equiv \sum_{i}^{n} c_i(t)\,|i\rangle\,, \tag{2.12}$$

being the $c_i(t)$ time-dependent complex amplitudes. The evolution in time of a quantum state from an initial state $|\Psi(t_0)\rangle$ at time t_0 is deterministic and can be described through the *Schrödinger equation* :

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \mathbf{H}(t) |\Psi(t)\rangle, \tag{2.13}$$

where $\hbar$ is Planck's fundamental constant, $t > t_0$, and $\mathbf{H}(t)$ is called the Hamiltonian operator, associated with the total energy of the system.

Alternatively, (2.13) can be written by defining the *evolution operator* $\mathbf{U}(t, t_0)$ by writing

$$|\Psi(t)\rangle = \mathbf{U}(t, t_0) |\Psi(t_0)\rangle. \tag{2.14}$$

The substitution of (2.14) into (2.13) therefore provides

$$i\hbar \frac{\partial}{\partial t} \mathbf{U}(t, t_0) = \mathbf{H}(t)\mathbf{U}(t, t_0). \tag{2.15}$$

In this thesis there will only be cases in which the Hamiltonian operator does not depend explicitly on time, we will then represent it simply by $\mathbf{H}$. Also, for simplicity, $\hbar = 1$ in this chapter and in the rest of this thesis. Taking this into consideration, integration of (2.15) gives

$$\mathbf{U}(t, t_0) = e^{-i\mathbf{H}(t-t_0)}. \tag{2.16}$$

$\mathbf{U}(t, t_0)$ is a unitary operator, since

$$\mathbf{U}^\dagger(t, t_0)\mathbf{U}(t, t_0) = \mathbb{I}. \tag{2.17}$$

In the following, we recall the discrete case described in the previous section where $\mathbf{H}$ is defined over a n-dimensional Hilbert space $\mathscr{H}$ - the extrapolation to the continuous case can be done straightforwardly through the use of integrals. The set of eigenvalues $e_1, e_2, ..., e_n$, constitutes the spectrum of $\mathbf{H}$, being the possible values for the total energy of the system. These eigenvalues are respectively associated with the eigenvectors $|e_1\rangle, |e_2\rangle, ..., |e_n\rangle$. Thus, $\mathbf{H}$ has the following diagonal representation

$$\mathbf{H} = \sum_i^n e_i |e_i\rangle \langle e_i|. \tag{2.18}$$

Thus, for an eigenstate $|e_i\rangle$, and from (2.16) and (2.18), one obtains

$$\mathbf{U}(t, t_0) |e_j\rangle = e^{-ie_j(t-t_0)} |e_j\rangle. \tag{2.19}$$

The eigenstates are therefore called *stationary* states, since systems initially in an eigenstate will remain in it at all times due to the fact that the effect of the dynamics upon them only adds a global phase, which cannot be observed. These global phases do not affect the probabilities of measuring each one of the eigenvalues of an observable (see next section).

2.1.4 Projective measurements

The process called a *measurement* within the context of quantum theory is particularly challenging to our intuition. In classical physics, measurements of physical systems can in principle be carried out with arbitrarily small disturbance on the system. As we will see, this does not hold for *quantum measurements*, which interpretation is far from intuitive: for an overview of the problems related to the interpretation of the quantum measurement, the so-called "quantum measurement problem", see Ref. [Leggett, 2005].

In quantum theory, when a measurement of a physical quantity associated with an observable $\mathbf{A}$ is performed, the obtained outcome is randomly determined at the time of the measurement out of its n eigenvalues. This process is known as *collapse*. The probability p_i of obtaining a particular eigenvalue λ_i when measuring $\mathbf{A}$, given that the system's normalized state is $|\Psi\rangle$, is

$$p_i = |\langle i \,|\, \Psi\rangle|^2, \tag{2.20}$$

where $|i\rangle$ is the normalized eigenstate corresponding to the eigenvalue λ_i. This postulate is called *Born rule*. Therefore, it connects the quantum state to what can be observed - for instance, as discussed above, the aforementioned probabilities can be associated with interference patterns.

In other words, (2.20) gives the probability p_i of projecting the system's state onto the eigenstate $|i\rangle$: since the result λ_i is obtained, the system's state is updated to $|i\rangle$. This process is named a *projective measurement*. This suggestive name is due to the fact that it can be represented through the definition of a *projector* $\mathbb{P}_\mathbf{i}$:

$$\mathbb{P}_i = |i\rangle \langle i| \,. \tag{2.21}$$

For instance, by acting the projector $\mathbb{P}_i$ upon the state $|\Psi\rangle$ of (5.9), given the orthonormality condition between the eigenstates of (2.5), one obtains

$$\mathbb{P}_i \,|\Psi\rangle = |i\rangle \langle i \,|\, \Psi\rangle = c_i \,|i\rangle \,. \tag{2.22}$$

One can notice that the following relation holds:

$$\sum_{i}^{n} \mathbb{P}_i = \sum_{i}^{n} |i\rangle \langle i| = \mathbb{I}. \tag{2.23}$$

Using the definition (2.21), the probability p_i (2.20) can therefore be rewritten as

$$p_i = \langle \Psi \,|\, \mathbb{P}_i \,|\, \Psi \rangle = \langle \Psi \,|\, i \rangle \langle i \,|\, \Psi \rangle = |c_i|^2. \tag{2.24}$$

Finally, after the realization of many measurements on several *copies* of systems prepared in the quantum state $|\Psi\rangle$ allowing one to collect some statistics, the *expected value* of the observable $\mathbf{A}$ can then be obtained, which is defined as follows

$$\langle \mathbf{A} \rangle \equiv \langle \Psi \,|\, \mathbf{A} \,|\, \Psi \rangle = \sum_{i}^{n} \langle \Psi \,|\, i \rangle \langle i \,|\, \mathbf{A} \,|\, i \rangle \langle i \,|\, \Psi \rangle = \sum_{i}^{n} p_i \lambda_i. \tag{2.25}$$

Now, once the observable $\mathbf{A}$ is measured and a particular eigenvalue λ_i obtained, the system's state is updated in accordance with the corresponding eigenstate $|i\rangle$:

$$|\Psi\rangle \to \frac{\mathbb{P}_i \,|\Psi\rangle}{\sqrt{\langle \Psi \,|\, \mathbb{P}_i \,|\, \Psi \rangle}} \equiv |i\rangle \,. \tag{2.26}$$

2.1.5 Density operator: pure and mixed states

So far we have used *pure* quantum states in order to introduce quantum formalism. Pure states are called *vector states* and can be represented by a ket, such as $|\Psi\rangle$.

Nevertheless, we use the pedagogical support introduced above to address realistic situations, in which it is impossible to perfectly attribute a pure state to quantum systems. Similar situations in classical physics are those in which the system's classical state cannot be perfectly known, the use of probabilities in order to write the *statistical* state of the physical system being necessary. For example, a thermodynamical system in equilibrium at temperature T has a probability proportional to $e^{E_n/kT}$ of being in a energy state E_n.

In quantum theory, this is expressed through a *statistical mixture* of pure states. This is the case when probabilities $f_1, f_2, ..., f_\nu$ are associated with the quantum states $|\psi_1\rangle\,, |\psi_1\rangle\,, ..., |\psi_\nu\rangle$ respectively. The representation of this general case is possible by defining the *density operator*.

Considering pure states $|\psi\rangle = \sum_i^n c_i |i\rangle$, one can define their correspondent density operators, ρ, as:

$$\rho \equiv |\psi\rangle \langle\psi| . \tag{2.27}$$

Thus, in the orthonormal basis of eigenstates $|i\rangle$, with a finite number of eigenstates n, the density operator has a matrix representation, its matrix elements being given by

$$[\rho]_{ij} = \langle i \,|\, \rho \,|\, j\rangle = c_i^* c_j. \tag{2.28}$$

As an example, for $n = 2$ and therefore

$$|\psi\rangle = c_1 |1\rangle + c_2 |2\rangle ,$$

the associated density operator ρ is

$$\rho = \begin{pmatrix} |c_1|^2 & c_1^* c_2 \\ c_1 c_2^* & |c_2|^2 \end{pmatrix} . \tag{2.29}$$

The probabilities $p_i = |c_i|^2$, the diagonal terms of ρ, are called *populations* of the eigenstates $|i\rangle$; the terms $c_i^* c_j$ are in turn called *coherences*, since the interference term K (2.3) is non-zero only if these crossed terms are also non-zero. Thus, one can verify quantum interference if the coherences are not equal to zero.

From the normalization condition, we know that it can be expressed in terms of ρ as follows:

$$\sum_i^n |c_i|^2 = \sum_i^n [\rho]_{ii} = \mathrm{Tr}\{\rho\} = 1. \tag{2.30}$$

Similarly, for the expected value (2.25):

$$\langle \mathbf{A} \rangle = \sum_i^n p_i \lambda_i = \mathrm{Tr}\{\rho \mathbf{A}\}, \tag{2.31}$$

where p_i is the probability associated with the obtention of the outcome λ_i when the system is measured.

The Schrödinger equation for the system's dynamics (2.13) can also be rewritten by using the definition of density operator:

$$i\frac{d}{dt}\rho(t) = [\mathbf{H}(t), \rho]. \tag{2.32}$$

Finally, the probabilities $p_i(t)$, which can be derived from (2.24), can be expressed as

$$p_i(t) = \mathrm{Tr}\{\rho(t)\mathbb{P}_i\}. \tag{2.33}$$

Thus, one can see that the density operator provides a characterisation of a system's quantum state, once one can obtain from it the same predictions as obtained from $|\psi\rangle$.

We will now analyse the situation where the system's state cannot be represented as a pure state, but rather as statistical mixture of pure states, given that the probabilities $f_1, f_2, ..., f_\nu$ are assigned to vector states $|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_\nu\rangle$, respectively. In order to simplify the notation, we omit the time t in the following - unless when deriving the system's dynamics from the dynamics of pure states. The system's state will be then generally represented as

$$\rho = \sum_k^\nu f_k |\psi_k\rangle \langle\psi_k|, \tag{2.34}$$

where the probabilities f_k satisfy

$$\sum_i^\nu f_k = 1. \tag{2.35}$$

Hence, the normalization of ρ will be given by

$$\mathrm{Tr}\{\rho\} = \sum_k^\nu f_k \mathrm{Tr}\{\rho_k\} = 1. \tag{2.36}$$

since $\mathrm{Tr}\{\rho_k\} = 1$.

The probability $p(\lambda_i)$ of obtaining the eigenvalue λ_i when measuring on the system will be generally given by

$$p(\lambda_i) = \sum_k^\nu f_k \mathrm{Tr}\{\rho_k \mathbb{P}_i\} = \mathrm{Tr}\{\rho\mathbb{P}_i\}. \tag{2.37}$$

Analogously, for the expected value,

$$\langle \mathbf{A} \rangle = \sum_{i}^{n} p(\lambda_i)\lambda_i = \mathrm{Tr}\{\rho \sum_{i}^{n} \lambda_i \mathbb{P}_i\} = \mathrm{Tr}\{\rho \mathbf{A}\}. \tag{2.38}$$

In order to derive the system's dynamics, we now write the density operator at time t as $\rho(t)$:

$$\rho(t) = \sum_{i}^{\nu} f_k \rho_k(t), \tag{2.39}$$

where $\rho_k(t)$ is given by (2.27). It follows then immediately from the linearity of (2.32) and (2.39) that

$$i\frac{d}{dt}\rho(t) = [\mathbf{H}(t), \rho]. \tag{2.40}$$

As before, the system's dynamics can be expressed in terms of the evolution operator $\mathbf{U}(t)$ (2.16). It can be verified from (2.14), (2.27) and (5.30) that the evolution of the system for this general case can also be written as

$$\rho(t) = \mathbf{U}^{\dagger}(t)\rho_0 \mathbf{U}(t), \tag{2.41}$$

where ρ_0 is the system's state at t_0, $\rho_0 = \rho(t_0)$.

Therefore, in general, a quantum system can be represented by a density operator ρ, *i. e.*, a positive hermitian operator.

2.1.6 Composite quantum systems: separable and entangled states

Consider two quantum systems $\mathcal{A}$ and $\mathcal{B}$ which are respectively associated with the Hilbert spaces $\mathscr{H}_{\mathcal{A}}$ and $\mathscr{H}_{\mathcal{B}}$, of dimensions $n_{\mathcal{A}}$ and $n_{\mathcal{B}}$, respectively. The Hilbert space $\mathscr{H}_{\mathcal{AB}}$ associated with the system constituted by these two *subsystems* or *parties* $\mathcal{A}$ and $\mathcal{B}$, which we will call the *global system* $\mathcal{A}+\mathcal{B}$, is defined through the tensor product of $\mathscr{H}_{\mathcal{A}}$ and $\mathscr{H}_{\mathcal{B}}$:

$$\mathscr{H} = \mathscr{H}_{\mathcal{A}} \otimes \mathscr{H}_{\mathcal{B}}. \tag{2.42}$$

The global system is therefore called a *composite* quantum system.

In order to simplify and better illustrate this, let us consider the case in which $\mathscr{H}$ is constituted only by the two parties $\mathscr{H}_{\mathcal{A}}$ and $\mathscr{H}_{\mathcal{B}}$. A global system's state $\rho \in \mathscr{H} = \mathscr{H}_{\mathcal{A}} \otimes \mathscr{H}_{\mathcal{B}}$ is then considered a *separable state* if it can be written as a convex sum of *product states*. Product states are defined as the tensor product of a state $\rho_{\mathcal{A}}$ of the system $\mathcal{A}$ and $\rho_{\mathcal{B}}$ of the system $\mathcal{B}$, that is

$$\rho = \rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}}. \tag{2.43}$$

In a similar way, for the pure states $|\psi\rangle_{\mathcal{A}}$ and $|\phi\rangle_{\mathcal{B}}$ respectively associated with each one of the parties $\mathcal{A}$ and $\mathcal{B}$, the separable global state can be written as $|\Psi\rangle = |\psi\rangle_{\mathcal{A}} \otimes |\phi\rangle_{\mathcal{B}}$, or more compactly, $|\Psi\rangle = |\psi_{\mathcal{A}}, \phi_{\mathcal{B}}\rangle = |\psi_{\mathcal{A}}\phi_{\mathcal{B}}\rangle$.

In what follows, we consider the case $n_{\mathcal{A}}$ be the dimension of $\mathscr{H}_{\mathcal{A}}$ and $n_{\mathcal{B}}$ the dimension of $\mathscr{H}_{\mathcal{B}}$ satisfying $n_{\mathcal{A}} = n_{\mathcal{B}} = 2$. This corresponds to two-level systems or *qubits* for instance, which have a basis formed of two eigenstates that we denote by $\{|0\rangle, |1\rangle\}$. Taking two qubits defined by this basis into consideration, the basis associated with $\mathscr{H}_{\mathcal{AB}}$ is then given by the tensor product of the eigenstates constituting the basis: $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

A separable global pure state in this basis is given, for instance, by

$$\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle) = \frac{1}{\sqrt{2}}|0\rangle \otimes (|0\rangle + |1\rangle). \tag{2.44}$$

However, one can have global states which do not admit a representation as separable states. As an example, one can write the following pure state, which is not separable:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle). \tag{2.45}$$

This state was named *entangled state* by Schrödinger [Schrödinger, 1935]. It establishes correlations between the system's parties which can be distinguished by a given measurement apparatus - this distinction between the system's parties is what allows the description of a quantum system as a composite quantum system. Entangled states are the *resource* of non-classical features of quantum mechanics such as nonlocality, as we will see later in this chapter. They are also fundamental in quantum information theory [Nielsen and Chuang, 2010], since many of its protocols are based on them.

2.1.7 Kraus operators and generalized measurements

In this section, we consider the definition of a *linear and completely positive map* $\mathcal{M}$ from $\mathscr{H}$ to $\mathscr{H}$. This means that given $\rho = \sum_k c_k \rho_k$ with $c_k \in \mathbb{C}$, the map $\mathcal{M}$ satisfies the following conditions:

$$\mathcal{M}\left(\sum_k c_k \rho_k\right) = \sum_k c_k \mathcal{M}(\rho_k) \tag{2.46}$$

$$\mathcal{M} \otimes \mathbb{I}_{\mathcal{E}} \geq 0. \tag{2.47}$$

Condition (2.47) requires $\mathcal{M}$ to be positive for any extension or *ancillary* $\mathscr{H}_{\mathcal{E}}$ of $\mathscr{H}$, where $\mathbb{I}_{\mathcal{E}}$ is the identity operator on $\mathscr{H}_{\mathcal{E}}$. The two conditions guarantee the preservation of the following properties of the density operator ρ by the map $\mathcal{M}$: linearity, positivity and hermicity. The application of $\mathcal{M}$ to ρ can be represented as

$$\mathcal{M}(\rho) = \sum_i^h = K_i^\dagger \rho K_i, \tag{2.48}$$

where the operators K_i are called *Kraus operators* and satisfy

$$\sum_i^h K_i^\dagger K_i = \mathbb{I}_{\mathcal{E}}, \tag{2.49}$$

where h is the dimension of $\mathcal{H}_{\mathcal{E}}$.

An important definition in the present context is the one of *reduced density operator*. In order to introduce it, let $\mathcal{S}$ be a system and $\mathcal{E}$ its ancillary. We also define $\mathbf{U}_{\mathcal{SE}}$ as a unitary evolution operator in $\mathscr{H}_{\mathcal{SE}} = \mathscr{H}_{\mathcal{S}} \otimes \mathscr{H}_{\mathcal{E}}$: the global system $\mathcal{S} + \mathcal{E}$ evolves unitarily with dynamics given by $\mathbf{U}_{\mathcal{SE}}$, and for that reason is called a *closed system*. Using $\mathbf{U}_{\mathcal{SE}}$, the evolution of a separable initial pure state at $t = 0$, $|\Psi_0\rangle = |\psi_{\mathcal{S}}\rangle \otimes |\phi_{\mathcal{E}}\rangle$, can be written such that the evolution of the system $\mathcal{S}$ will be represented by a Kraus map:

$$|\Psi(t)\rangle = \mathbf{U}_{\mathcal{SE}}(|\psi_{\mathcal{S}}\rangle \otimes |\phi_{\mathcal{E}}\rangle) = \sum_i^h (K_i \otimes \mathbb{I}_{\mathcal{E}})(|\psi_{\mathcal{S}}\rangle \otimes |i\rangle), \tag{2.50}$$

where $|i\rangle$ is an orthonormal basis for $\mathscr{H}_{\mathcal{E}}$. In terms of the initial global system's density operator $\rho_{\mathcal{SE}}(0) = |\Psi_0\rangle \langle\Psi_0|$ and with $\rho_{\mathcal{S}}(0) = |\psi_{\mathcal{S}}\rangle \langle\psi_{\mathcal{S}}|$ being the density operator of the system $\mathcal{S}$, the global system's state at time t, $\rho_{\mathcal{S}\mathcal{E}}(t) = |\Psi(t)\rangle\langle\Psi(t)|$, will read

$$\rho_{\mathcal{S}\mathcal{E}}(t) = \mathbf{U}^{\dagger}_{\mathcal{S}\mathcal{E}}(\rho_{\mathcal{S}} \otimes |\phi\rangle\langle\phi|_{\mathcal{E}})\mathbf{U}_{\mathcal{S}\mathcal{E}} = \sum_{i,w}(K_i \otimes \mathbb{I}_{\mathcal{E}} |\psi_{\mathcal{S}}, i\rangle\langle\psi_{\mathcal{S}}, w| K_i^{\dagger} \otimes \mathbb{I}_{\mathcal{E}}). \tag{2.51}$$

The evolved state $\rho_{\mathcal{S}}(t)$ of the system $\mathcal{S}$ itself, then, can be obtained from the global state (2.51), which evolves unitarily, by taking the *partial trace* over $\mathcal{E}$, i.e

$$\begin{aligned}\rho_{\mathcal{S}}(t) = \mathrm{Tr}_{\mathcal{E}}\{\rho(t)\} &= \sum_j \langle j| \left(\sum_{i,w}(K_i \otimes \mathbb{I}_{\mathcal{E}} |\psi_{\mathcal{S}}, i\rangle\langle\psi_{\mathcal{S}}, w| K_i^{\dagger} \otimes \mathbb{I}_{\mathcal{E}})\right)|j\rangle \\ &= \sum_j \langle j\,|\,i\rangle\langle w\,|\,j\rangle\,(K_i^{\dagger}(|\psi_{\mathcal{S}}\rangle\langle\psi_{\mathcal{S}}|)K_i) \\ &= \sum_j K_j^{\dagger}(|\psi_{\mathcal{S}}\rangle\langle\psi_{\mathcal{S}}|)K_j. \end{aligned} \tag{2.52}$$

One can therefore obtain the system's state $\rho_{\mathcal{S}}(t)$ from the global system's state $\rho(t)$ by tracing out the *ancillary* system $\mathcal{E}$. Thus, the state $\rho_{\mathcal{S}}(t)$ obtained this way is called reduced density operator.

Now if $\mathcal{M}$, in addition to linear and completely positive, is also *trace preserving*, i. e.

$$\mathrm{Tr}\{\mathcal{M}(\rho)\} = \mathrm{Tr}\{\rho\}, \tag{2.53}$$

then all the properties of the density operator $\rho_{\mathcal{S}}$ will be preserved by the map (linearity, positivity, hermiticity and trace). In this way, trace preserving Kraus operators provide a general description for quantum dynamics, including the cases in which the system's dynamics $\mathcal{S}$ is non-unitary due to its interaction with an ancillary system $\mathcal{E}$, as for the so-called *open quantum systems* [Zurek, 2003]. However, a unitary evolution can also be described by a Kraus map with $h = 1$ in (2.48) and $K_1 = \mathbf{U}$, as one can see by comparing (2.48) to (2.41).

In what follows, we recall the discussion about quantum measurements introduced in a previous section of this chapter. Here we introduce a general description of the *measurement process* described by Kraus operators. Hence, as we will see, a projective measurement is a particular case within this general framework. In order to present this generalization, let us consider the operators M_i instead of projectors $\mathbb{P}_i$, which are not necessarily hermitians and satisfy

$$\sum_i M_i^\dagger M_i = \mathbb{I}. \tag{2.54}$$

Then, one can write the probability p_i of obtaining a result i when a generalized measurement is realized by using the operators M_i as follows

$$p_i = \left\langle \psi \,\middle|\, M_i^\dagger M_i \,\middle|\, \psi \right\rangle, \tag{2.55}$$

where $|\psi\rangle$ is the system's state when the measurement is performed. As a result of the measurement, the system's state will be projected onto the following state:

$$|\psi\rangle \to |\psi_i\rangle = \frac{M_i\,|\psi\rangle}{\sqrt{p_i}}. \tag{2.56}$$

In a similar way, for a statistical mixture ρ, the probability p_i reads

$$p_i = \mathrm{Tr}\{\rho M_i^\dagger M_i\}, \tag{2.57}$$

and the state after the measurement will be given by

$$\rho \to \rho_i = \frac{M_i \rho M_i^\dagger}{p_i}. \tag{2.58}$$

From this we can define *Positive Operators Valued Measure* (POVM) as the set of n operators $E_i \equiv M_i^\dagger M_i$. The set E_i is constituted of hermitian ($E_i = E_i^\dagger$) and positive operators, $E_i > 0$, satisfying $\sum_i E_i = \mathbb{I}$. The probabilities p_i of obtaining the result associated with the element E_i is, in terms of these operators, given by

$$p_i = \mathrm{Tr}\{E_i \rho\}. \tag{2.59}$$

In the particular case where M_i is hermitian, we have $M_i = M_i^\dagger = \sqrt{E_i}$, and therefore after the measurement and obtention of the result associated the element E_i, the system's state becomes

$$\rho \to \rho_i = \frac{\sqrt{E_i}\rho\sqrt{E_i}}{p_i}. \tag{2.60}$$

The case of projective measurements is a particular case of POVM with $E_i = \mathbb{P}_i$. However, any POVM with n elements acting on a Hilbert space of dimension N can be written as a projective measurement on a Hilbert space of dimension $n > N$. This is the content of the *Neumark dilation theorem*.

2.2 Contextuality of quantum theory

2.2.1 (Non)contextuality

In this section we introduce the concept of *(non)contextuality*. Generally, the concept of contextuality is introduced as the dependence of probabilities of measurement outcomes on the *context*, which we precisely define in the present section. The contextuality of quantum theory, as demonstrated by Kochen-Specker theorem [Kochen and Specker, 1967] and developed in many other works [Laversanne-Finot et al., 2017, Winter, 2014, Kleinmann et al., 2012, Cabello, 2008, Cabello et al., 2015, Asadian et al., 2015, Amselem et al., 2009, Spekkens, 2005], shows the impossibility of a *non-contextual hidden variable* explanation of the predictions of quantum mechanics.

In the following, we will focus on the general operational framework introduced by Spekkens [Spekkens, 2005]. Within this framework, as we will see, an operational definition of *noncontextual operational models* and context are provided, through which several manifestations of (non)contextuality are identified.

Noncontextual ontological models for quantum theory

We first review an operational approach [Peres, 1993, Kraus, 1983, P. Busch and Lahti, 1995] which later in this chapter will applied to quantum theory [Spekkens, 2005]. In a laboratory, an experiment can be divided into the following procedures: *preparation*, *transformation* and *measurement*. Therefore, the probabilities of obtaining the different outcomes k associated with a given preparation preparation P, transformation T and measurement M can be written as $p(k|P, T, M)$. One may consider the transformation T as part of the preparation P: in this case, the probabilities are writen as $p(k|P, M)$. Different *equivalence classes* can then be defined: two preparations P_1 and P_2 are defined as equivalent if the probabilities for the different outcomes are the same for any transformation and measurement, i. e.

$$p(k|P_1, T, M) = p(k|P_2, T, M), \forall T, \tag{2.61}$$

Similarly, two transformations T_1 and T_2 are equivalent if

$$p(k|P, T_1, M) = p(k|P, T_2, M), \forall P, M, \tag{2.62}$$

and the same holds for two measurements M_1 and M_2:

$$p(k|P, T, M_1) = p(k|P, T, M_2), \forall P, T, \tag{2.63}$$

Suppose now that the equivalence class of a given experiment is specified. All the other features of the experiment, i.e., the ones which cannot be fixed by the specification of the equivalence class, constitute the experimental *context*.

Example of context described in Ref [Spekkens, 2005]. In an experiment for measuring photon polarization, one has 4 measurement procedures $\{M_1, M_2, M_3, M_4\}$ at one's disposal. The first measurement, M_1, is realized by a device as a piece of polaroid which permits the passage of vertically polarized light in the $\hat{z}$-axis, with a photodetector placed after it. The device associated with the measurement M_2 is in turn a birefringent crystal which separates the vertical polarized light in the z-axis from the horizontal components, followed by a photodetector oriented in the $\hat{z}$-axis output. This is represented in Fig. 2.2(a). The same description is valid for M_3 and M_4, which are the same as M_1 and M_2 respectively, except for the fact that they are performed with respect to an $\hat{n}$-axis, tilted with respect to $\hat{z}$, as it is represented in Fig. 2.2(b). In this way, the probabilities for the outcomes for M_1 are the same as for M_2 for all preparations, and the ones for M_3 are identical those for M_4. Notwithstanding, the probabilities for the outcomes for M_1 and M_2 are different from the probabilities for the outcomes for M_3 and M_4. The first pair of measurements belongs to an equivalence class, and the second pair to a different one. Therefore, the polaroid and the birefringent crystal's orientation define the different equivalence classes. However, the question of whether one uses the polaroid or the crystal does not change the equivalence class. This feature is therefore part of the context of the measurement.

Before moving on, we should also define an *ontological model*. An ontological model assumes that physical systems which are the subject of an experimental realization have definite properties irrespective of what is

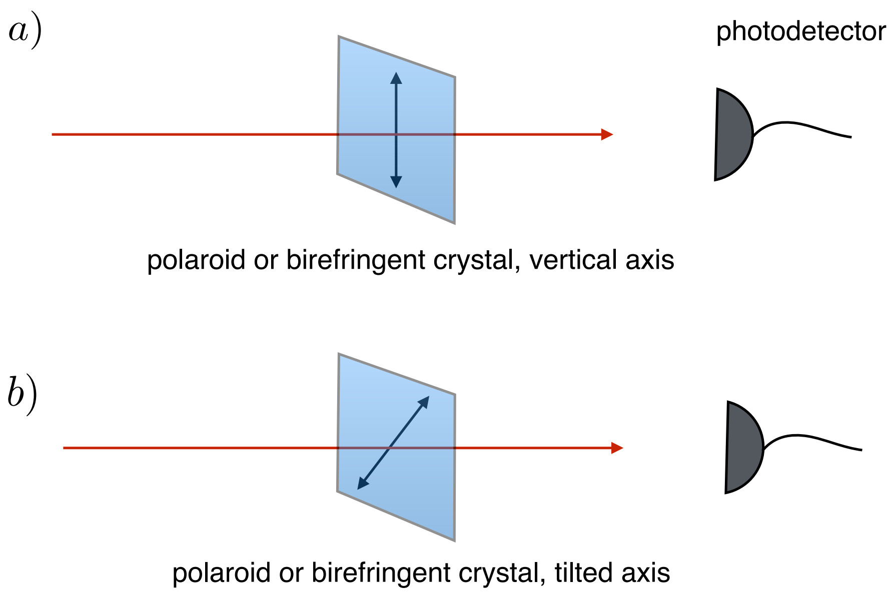

Figure 2.2: Representation of the different equivalence classes defined by the orientation of the polaroid (or birefringent crystal) in parts *a)* and *b)*, through which light is sent. In this way, in *a)*, one has the equivalence class defined by vertical ($\hat{z}$-direction) transmission axis. Analogously, in *b)* one has another equivalence class, defined by a tilted transmission axis. Using a polaroid or a birefringent crystal with the same axis orientation does not change the probabilities of obtaining the different results within a given experiment, and therefore does not change the equivalence class: these elements are, therefore, part of the context of the measurement.

known about the system, and that the specification of these properties at a given time describe its real or *ontic* state. If one cannot fully specify the ontic state of a system after the preparation procedure, then supplemental variables named *hidden variables* are required for the complete specification. The complete set of variables in an ontological model is characterized by λ, and the space of values of λ represented by Ω.

When considering an ontological model, one therefore assumes that preparations prepare ontic states. The same holds for measurements and transformations: in an ontological model, these terms refer to measurements and transformations of ontic states. Therefore, given a system prepared following a preparation procedure P, we can define the probability density $\mu_P(\lambda)$ over the variable λ. Thus, the preparation P prescribes probabilities to different ontic states λ.

In a similar way, we can associate the probability $\xi_{M,k}(\lambda)$ of obtaining a specific outcome k in a measurement M when the system is in the ontic state λ. This probability is called the *response function*. For a transformation T, we can write $\Gamma_T(\lambda', \lambda)$ as the probability density of this transformation leading the ontic state λ to the ontic state λ'.

We can then write the probability $p(k|P, T, M)$ of obtaining an outcome k given a preparation P, a transformation T and a measurement M:

$$p(k|P, T, M) = \int d\lambda' d\lambda \xi_{M,k}(\lambda') \Gamma_T(\lambda', \lambda) \mu_P(\lambda). \tag{2.64}$$

Let us now define a noncontextual ontological model as a model wherein the experimental realization depends only on its equivalence class: there is no dependence on the context. In this way, one can characterize ontological models according to the different equivalence classes. For instance, an ontological, *preparation noncontextual* model is such that

$$\mu_P(\lambda) = \mu_{e(P)}(\lambda). \tag{2.65}$$

where $e(P)$ is the equivalence class of the preparation P. Therefore, the density probabilities for preparations P associated with a ontic state λ depends only on the equivalence class $e(P)$. Similarly, an ontological, *measurement noncontextual* model satisfies

$$\xi_{M,k}(\lambda) = \xi_{e(M),k}(\lambda), \tag{2.66}$$

where $e(M)$ is the equivalence class of the measurement M. If in turn an ontological model is *transformation noncontextual*, the following condition is fulfilled:

$$\Gamma_T(\lambda', \lambda) = \Gamma_{e(T)}(\lambda', \lambda), \tag{2.67}$$

$e(T)$ being the equivalence class of the transformation T.

Thus, an ontological model which is noncontextual for all experimental procedures, i.e., preparations, transformations and measurements, is called *universally noncontextual*.

Let us now apply this operational approach to quantum theory. An equivalence class of preparations P in quantum theory is associated with a density operator ρ over the Hilbert space $\mathscr{H}$. Thus, if one assumes preparation noncontextuality in quantum theory, it implicates that the probability density associated with a preparation P depends solely on ρ:

$$\mu_P(\lambda) = \mu_\rho(\lambda). \tag{2.68}$$

An equivalence class of a transformation T is associated with completely positive maps $\mathcal{T}$. Therefore, the assumption of transformation noncontextuality in quantum theory implies that the probability density associated with a transformation T of the ontic state λ' to the ontic state λ depends uniquely on the completely positive map $\mathcal{T}$, that is

$$\Gamma_T(\lambda', \lambda) = \Gamma_{\mathcal{T}}(\lambda', \lambda). \tag{2.69}$$

Finally, an equivalence class of a measurement is associated with a POVM $\{E_k\}$. Accordingly, measurement noncontextuality in quantum theory requires that the set of response functions[3] be dependent only on the POVM $\{E_k\}$:

$$\xi_{M,k}(\lambda) = \xi_{\{E_k\},k}(\lambda). \tag{2.70}$$

2.2.2 Bell inequality and locality

Local-causality or *locality* is the notion according to which two physical systems can only obtain information from each other if there is an interaction between them. Furthermore, two quantum systems can only interact locally. Otherwise, the system is called *nonlocal*.

We recall the phenomenon of entanglement previously introduced in this chapter, which can be verified for quantum systems possessing two or more parts. As it can be seen from the state in (2.45), measuring one of the system's parties in state $|0\rangle$ ($|1\rangle$) implies that the second party *collapses* into state $|0\rangle$ ($|1\rangle$). In the case that the system's parties are far away, it necessarily follows that the phenomenon of entanglement defies the notion of locality. Indeed, the observation of nonlocality implies entanglement, leading to the empirical inadequacy of locally-causal theories [O. J. E. Maroney, 2014].

[3] As a matter of fact, this is a generalized notion of measurement contextuality corresponding to *objectively indeterministic* ontological models, since it involves *probabilities* of different outcomes for a given ontic state instead of the outcomes themselves.

In a famous 1935 paper by Einstein, Podolsky and Rosen, the authors consider the following definition for the *completeness* of a physical theory [Einstein et al., 1935]

> *Every element of the physical reality must have a counterpart in the physical theory. We shall call this the condition of completeness.*

Given this definition, they showed that quantum theory is incomplete, *i.e.*, incompatible with the description of completeness above, and concluded with the following statement,

> *While we have thus shown that the wave function does not provide a complete description of the physical reality, we left open the question of whether or not such description exists. We believe, however, that such a theory is possible.*

This question remained open until the formulation of Bell theorem in 1964 [Bell, 1964,Bell, 2004]. Bell considered a mathematical formulation of the assumption of realism and locality in terms of *hidden variables*. Accordingly, the assumption of *realism* (*i.e.*, that physical quantities have definite values at all times, whether they are measured or not) would imply that, if correlations between systems far away from each other are verified, these correlations could only have been established before the measurements on those systems take place. Furthermore, the assumption of local-causality would in turn imply that, before the measurement, the distant systems could only have communicated through the hidden variables λ. In this way, one would have a physical theory wherein there would be no need to speak of nonclassical concepts such as entanglement. Based on these assumptions, inequalities which consists of a sum of spatial correlations between two distant systems, called *Bell inequalities*, were derived. The experimental violation of such inequalities accounts, therefore, for a violation of local realism.

For instance, one of these inequalities is known as the *Clauser-Horne-Shimony-Holtz (CHSH) inequality* [Clauser et al., 1969]. Consider a system $\mathcal{S}$ constituted of a party $\mathcal{A}$, to which is associated the dichotomic observables A_1 and A_2, and a party $\mathcal{B}$, to which in turn one associates the dichotomic observables B_1 and B_2. The CHSH inequality is then expressed as

$$K_{CHSH} = \langle A_1 B_1 \rangle + \langle A_1 B_2 \rangle + \langle A_2 B_1 \rangle - \langle A_2 B_2 \rangle \leq 2, \tag{2.71}$$

where

$$\langle A_i B_j \rangle = \int x_i y_j p(x_i, y_j | A_i, B_j) dx_i dy_j. \tag{2.72}$$

In the expression of the correlation above, x_i, y_j are respectively the outcomes associated with the observables A_i, B_j, where $p(x_i, y_j|A_i, B_j)$ is the probability of obtaining these outcomes when measuring A_i, B_j.

As a result, any quantum state violating the inequality (2.71) cannot be explained by a local hidden variable model.

Experimental tests of Bell-type inequalities

The derivation of CHSH inequalities was crucial for the development of experimental tests of Bell-type inequalities. Indeed, the first test of Bell-type inequality was carried out by Freedman and Clauser in 1972, showing the violation of a variant of the CHSH inequality [Freedman and Clauser, 1972]. The system used in this first test was constituted of a pair of photons with entangled polarization.

Notwithstanding the observation of violation in this first experiment, it is important to mention that it was subject to *detection* and *locality loopholes*. The detection loophole has as its cause an additional assumption called *fair sample assumption*. This means that only a small fraction of probes are detected (less than $\frac{2}{3}$ of the pairs), and it is assumed that this is a representative sample of the total number of probes.

The second loophole, the locality one, is the assumption that measurements are performed without the possibility of communication between the two spots where they are carried out. Practically, this is ensured by a measurement duration short enough to avoid that any signal travels with the speed of light from one spot to the other. Remarkably, this loophole was already overcame in 1982 Aspect's experiment [Aspect et al., 1982a]. This experiment and many other tests were also realized considering entangled-polarized photons systems [Aspect et al., 1981, Giustina et al., 2015, Giustina et al., 2013, Hensen et al., 2015]. However, all these realizations were subjected to loopholes.

The realization of a free-loophole Bell test, closing both the detection and locality loopholes, was only very recently reported by using distant (separation of 1.3 km) entangled electron spins [Hensen et al., 2015].

2.2.3 Leggett-Garg inequality and noninvasiveness

In 1985, Leggett and Garg derived an inequality based on two assumptions which in the authors' words were expressed as follows:

(i) Macroscopic realism: a macroscopic system with two or more macroscopically distinct states available to it will at all times be in one of those states.

(ii) Noninvasive measurability: it is possible, in principle, to determine the state of the system with arbitrarily small perturbation to its subsequent dynamics.

At this point, before proceeding, it is important to clarify the fact that Leggett and Garg's original motivation for the proposition of the Leggett-Garg inequality was the question of whether quantum theory can be extrapolated to the macroscopic world [Leggett, 2002], which would allow one to witness its nonclassical effects involving objects in the scale of our everyday lives, for instance. In particular, this fact becomes clear in the following Leggett and Garg's statement [Leggett and Garg, 1985], when referring to assumptions *(i)* and *(ii)* above:

A direct extrapolation of quantum mechanics to the macroscopic level denies this [assumptions *(i)* and *(ii)*].

This is the reason why the authors call the assumption (i) *macroscopic realism* instead of *realism*, and refer, in their statement of assumption *(i)*, to a "macroscopic system". This assumption can also be seen as an implicit way of referring to the classical world, since macroscopic objects are intuitively expected to have their behaviour described by classical physics. However, regardless of the use of the term "macroscopic" to name the assumption of macroscopic realism in Leggett and Garg's statement, this assumption can be reformulated and called *realism*, in the following way:

Realism: a system with two or more distinct states available to it will at all times be in one of those states.

Indeed, this would be a clearer statement of assumption *(i)*, highlighting the fact that this assumption refers to the notion of realism, and can be considered independently of the size of the system subjected to a Leggett-Garg test. Irrespective of this fact, following Leggett and Garg, this assumption is commonly called macroscopic realism in the literature, even for propositions or experimental tests of the Leggett-Garg inequality involving microscopic systems [Emary et al., 2014]. See chapter 5 for a description of some protocols for experimental tests of the Leggett-Garg inequality.

As we will see in details in the derivation below, the Leggett-Garg inequality involves measurements of a two-valued observable Q that may be associated with physical properties of a system at different times, such that $Q_i = Q(t_i)$. By considering experimental realizations in which a system initially at t_0 evolves in time, and by measuring Q at two different times in order to obtain the temporal correlations $\langle Q_k Q_l \rangle$, an example of Leggett-Garg inequality is given by

$$-1 \leq K_{LG} \equiv \langle Q_1 Q_2 \rangle + \langle Q_2 Q_3 \rangle - \langle Q_1 Q_3 \rangle \leq 1. \tag{2.73}$$

Accordingly, the Leggett-Garg inequality violation would imply the violation of at least one of these assumptions.

However, the Leggett-Garg inequality derivation can be based solely on the notion of noninvasive measurability. By following Ref. [O. J. E. Maroney, 2014], we demonstrate that a condition based on this assumption, called *measurement noninvasiveness*, is sufficient for the Leggett-Garg inequality derivation. Indeed, as pointed out by Maroney and Timpson [O. J. E. Maroney, 2014], whether the assumption of macroscopic realism can be ruled out by the Leggett-Garg inequality violation or not is the subject of a debate which started as early as 1987 [Ballentine, 1987, Leggett and Garg, 1987, Leggett, 1988]. Given this, we will also discuss how the assumption of macroscopic realism can be tested by the Leggett-Garg inequality, and therefore, how it can be connected to the notion of noninvasive measurability, to which we will refer as *(measurement) noninvasiveness*.

Leggett-Garg inequality derivation

We first consider the following experimental realization: a system $\mathcal{S}$ is prepared according to a preparation procedure P at time t_0. In the following description, we consider measurements of a two-valued quantity $Q = \pm 1$. A first measurement M_1 which has the two possible outcomes $Q_1 = \pm 1$ is performed on $\mathcal{S}$ at time $t_1 > t_0$. $\mathcal{S}$ is then subjected to the transformation T_1 between times t_1 and $t_2 > t_1$. At t_2, a measurement M_2 which also has two possible outcomes $Q_2 = \pm 1$ is done on S. Finally, between t_2 and $t_3 > t_2$, $\mathcal{S}$ undergoes a transformation T_2, and then at t_3 one performs a last two-valued measurement M_3, with possible outcomes $Q_3 = \pm 1$. According to the operational approach introduced above, one can represent the joint probability distribution associated with this experimental realization as follows:

$$p_{(P,M_1,T_1,M_2,T_2,M_3)}(Q_1 = q_i, Q_2 = q_j, Q_3 = q_k). \tag{2.74}$$

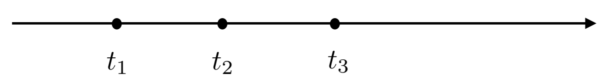

Figure 2.3: The probability $p_{(P,M_1,T_1,M_2,T_2,M_3)}(Q_1 = q_i, Q_2 = q_j, Q_3 = q_k)$ (of obtaining the outcome $Q_1 = q_i$ when measuring the system at the subsequent times t_1 (measurement M_1), $Q_2 = q_j$ at t_2 (measurement M_2) and $Q_3 = q_k$ at t_3 (measurement M_3)) is associated with experimental realizations in which all three measurements M_1, M_2 and M_3 are carried out in each run of the experiment. The realization of these measurements is represented by the dots over the "arrow of time" line.

Suppose now that one can derive probabilities[4] associated with a smaller number of variables by taking the marginal over the joint probability distribution of (2.75), for instance

$$p_{(M_1,M_2,M_3)}(Q_1 = q_i) = \sum_{q_j q_k} p_{(M_1,M_2,M_3)}(Q_1 = q_i, Q_2 = q_j, Q_3 = q_k). \tag{2.75}$$

One can then write the correlations $\langle Q_1 Q_2 \rangle_{M_1 M_2 M_3}$ between the outcomes of measurements realized at times t_1 and t_2, given that all three measurements were performed, as

$$\langle Q_1 Q_2 \rangle_{M_1 M_2 M_3} = \sum_{q_i q_j} p_{(M_1,M_2,M_3)}(Q_1 = q_i, Q_2 = q_j) q_i q_j. \tag{2.76}$$

Let us consider the definition of the following quantity:

$$\langle Q_{LG} \rangle_{M_1 M_2 M_3} \equiv \langle Q_1 Q_2 \rangle_{M_1 M_2 M_3} + \langle Q_2 Q_3 \rangle_{M_1 M_2 M_3} - \langle Q_1 Q_3 \rangle_{M_1 M_2 M_3}. \tag{2.77}$$

[4]For simplicity, we omit the index for the preparation and transformations from now on.

Assuming that all three measurements are performed, one can see from (2.75) and (2.76) that $\langle Q_{LG}\rangle_{M_1M_2M_3}$ satisfies

$$-1 \leq \langle Q_{LG}\rangle_{M_1M_2M_3} \leq 1. \tag{2.78}$$

Thus, the bound of (2.78) will *always* be fulfilled, even within quantum theory: it does not matter whether one previously had the information of these values, in which case they are merely revealed by the measurements, or whether these values are defined as a consequence of performing the measurements.

In what follows, we analyse the realizations in which only two measurements out of three possible (M_1, M_2, M_3) are performed. Similarly, we consider the quantity

$$K_{LG} \equiv \langle Q_1Q_2\rangle_{M_1M_2} + \langle Q_2Q_3\rangle_{M_2M_3} - \langle Q_1Q_3\rangle_{M_1M_3}, \tag{2.79}$$

where the correlations can be written, for instance, as

$$\langle Q_1Q_2\rangle_{M_1M_2} = \sum_{q_iq_j} p_{(M_1,M_2)}(Q_1 = q_i, Q_2 = q_j)q_iq_j. \tag{2.80}$$

The other correlation terms in (2.79) can be similarly written.

Let us then suppose that the probabilities associated with these realizations can be obtained by taking the marginals of the joint probability (for which the 3 measurements are performed):

$$p_{(M_1,M_2)}(Q_1 = q_i, Q_2 = q_j) = \sum_{q_k} p_{(M_1,M_2,M_3)}(Q_1 = q_i, Q_2 = q_j, Q_3 = q_k), \tag{2.81}$$

$$p_{(M_2,M_3)}(Q_2 = q_j, Q_3 = q_k) = \sum_{q_i} p_{(M_1,M_2,M_3)}(Q_1 = q_i, Q_2 = q_j, Q_3 = q_k), \tag{2.82}$$

$$p_{(M_1,M_3)}(Q_1 = q_i, Q_3 = q_k) = \sum_{q_j} p_{(M_1,M_2,M_3)}(Q_1 = q_i, Q_2 = q_j, Q_3 = q_k). \tag{2.83}$$

We stress the fact that the probabilities $p_{(M_1,M_2)}(Q_1 = q_i, Q_2 = q_j)$, $p_{(M_2,M_3)}(Q_2 = q_j, Q_3 = q_k)$ and $p_{(M_1,M_3)}(Q_1 = q_i, Q_3 = q_k)$ refer to three different and independent experimental realizations, in which the measurements are performed only at two out of the predefined times t_1, t_2 and t_3, considering the same preparation and transformations used in order to obtain (2.75). For this reason, it is not trivial that the probabilities asso-

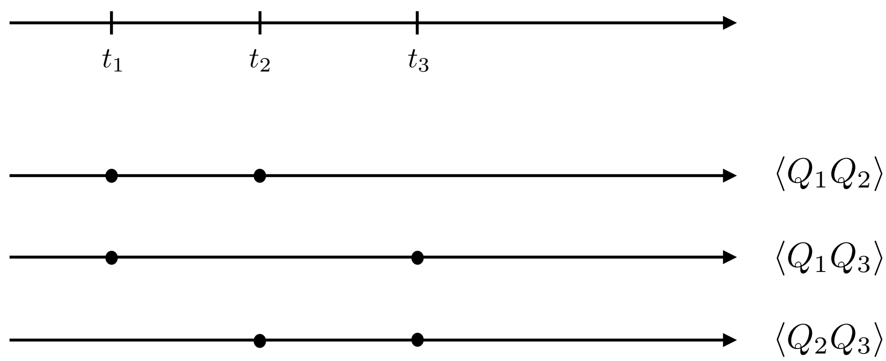

Figure 2.4: In order to determine the two-time correlations $\langle Q_l Q_m \rangle$, one performs a a measurement at time t_l, of which result is $Q_l = q_l$ and then a measurement at a later time t_m, of which result is $Q_m = q_m$. As before, we indicate the instant of time at which the measurement is carried out by a dot over the "arrow of time" line.

ciated with the experiments involving just two measurements are related to the experiment wherein one realizes all three measurements as made explicit in (2.81), (2.82) and (2.83). However, if one can derive $p_{(M_1,M_2)}$, $p_{(M_2,M_3)}$ and $p_{(M_1,M_3)}$ from the joint probability, which is associated with an experiment in which all the three measurements are performed, one can conclude that there must be no difference for these probabilities within the experimental realizations in which all three measurements M_1, M_2 and M_3 are performed and those in which one skips one of the measurements M_1, M_2 or M_3. The following conclusion can be therefore drawn:

If the probabilities $p_{(M_1,M_2)}(Q_1 = q_i, Q_2 = q_j)$, $p_{(M_2,M_3)}(Q_2 = q_j, Q_3 = q_k)$ and $p_{(M_1,M_3)}(Q_1 = q_i, Q_3 = q_k)$ (which are associated to experimental realizations wherein only the two measurements to which they refer are performed out of the three measurements M_1, M_2 and M_3) can be obtained by taking the marginal distribution of the joint probability $p_{(M_1,M_2,M_3)}(Q_1 = q_i, Q_2 = q_j, Q_3 = q_k)$, then one can conclude that it is indifferent whether one performs all the three measurements or just a smaller set of them in an experimental realization. In this case, the Leggett-Garg inequality (2.79) will hold, and the measurements can therefore be called noninvasive.

Formalizing operational noninvasiveness

We can therefore formalize the operational notion of noninvasive measurability of the previous section, within the context of the operational approach presented before. Let us consider a preparation P, and a measurement M followed by the measurement M'. We define the measurement M as *operationally noninvasive* for the preparation P and subsequent measurement M' if it is impossible to state if M was performed based on the observed statistics of P and M', i. e.,

$$p_{(P,M')}(Q' = q_j) = \sum_{q_i} p_{(P,M,M')}(Q = q_i, Q' = q_j). \tag{2.84}$$

This is the notion of noninvasiveness which is verified by conditions (2.82) and (2.83). If both conditions are not satisfied, then measurements M_1 and M_2 are operationally invasive. Condition (2.81) can be called in turn *no-signaling backwards in time*, since it dictates that measurements performed afterwards must not affect the statistics of previously performed measurements.

How can measurement noninvasiveness be connected to realism?

We based the Leggett-Garg inequality derivation uniquely on the operational notion of noninvasive measurabililty defined above, which can be viewed as a reformulation of assumption *(ii)* of Leggett and Garg's original proposition. Indeed, this is the assumption which can always be ruled out by a test of the Leggett-Garg inequality. Therefore, what is primarily witnessed by a Leggett-Garg inequality violation is that M_1 or M_2, or both, are operationally disturbing or invasive for their corresponding preparations and transformations.

When it comes to realism, one can first notice that the assumption of (macro)realism cannot be stated without the specification of the interpretation of quantum theory which one takes into consideration. For example, consider the framework of the de Broglie-Bohm theory [de Broglie, 1923, Bohm and Hiley, 1993]. Therefore, within the context of this theory, the assumption *(ii)* as stated by Leggett and Garg [Leggett and Garg, 1985], has no meaning, since quantum superpositions already have an ontological status.

Indeed, since the assumption of (macro)realism can be interpreted as the imposition of the prohibition of superposition of states, a question one might naturally ask is is the following: with respect to which basis are superpositions of states being tested by the Leggett-Garg inequality? In what follows, we will clarify this point by introducing the definition of *operational eigenstate mixture (macro)realism* [O. J. E. Maroney, 2014], which can be viewed as a refinement of Leggett and Garg's notion of (macroscopic) realism. We will see how this refined notion of (macroscopic) realism can be connected to noninvasiveness and therefore be dismissed by the Leggett-Garg inequality violation.

To introduce the definition of *operational eigenstate*, consider the operational framework described above. Let $e(M)$ be an equivalence class of measurements, with $M' \in e(M)$, where M' are measurements of a quantity $\tilde{Q}$. An operational eigenstate is defined as a particular equivalence class of preparations P which, when followed by any measurement $M' \in e(M)$, has either the probability 0 or 1 associated with the measurement outcomes q_i of $\tilde{Q}$. In this way, if one prepares the operational eigenstate q_i of $\tilde{Q}$, it then follows that any measurement $M' \in e(M)$ will give the outcome q_i with probability 1. Given this, noninvasiveness is verified if there is some measurement M within the operational equivalence class which is operational noninvasive when the system's state corresponds to an operational eigenstate of the quantity $\tilde{Q}$.

This is the motivation for the definition of *operational eigenstate mixture (macro)realism*, which accounts for the following view: *the only possible preparation states of a system S are operational eigenstates of $\tilde{Q}$ and their statistical mixtures.*

In order to formalize this notion, consider a preparation P_{q_i} which lies on the operational eigenstate equivalence class $\tilde{P}_{q_i}$, and which satisfies $p_{(P_{q_i},M)}(Q = q_i) = 1$ for all $M \in e(M)$. Let Ω be the space of ontic states λ, and the probability density associated with the preparations P_{q_i} given by $\mu_{P_{q_i}}(\lambda)$. Correspondingly, for all λ and $M \in e(M)$, the response function associated with λ is given by $\xi_M(Q = q_i|\lambda) = 1$. Let μ_{q_i} be a convex sum of operational eigenstate preparation densities $\mu_{P_{q_i}}$. As a result, every ontic state λ, to which μ_{q_i} is associated, is noncontextually value-definite with value $Q = q_i$.

In summary, if a measurement M_1 is operationally noninvasive for operational eigenstate preparations, then the statistics for (P, M_1, M_2) will not differ from those for (P, M_2). Therefore, if one does prove the invasiveness of M_1 by, for instance violating the Leggett-Garg inequality, then operational eigenstate mixture (macro)realism *must* be dismissed. It turns out then that invasiveness can be connected to the view of operational eigenstate (macro)realism.

2.2.4 The no-signaling in time condition

Kofler and Brukner proposed the no-signaling in time condition as a alternative to Leggett-Garg inequalities in Ref. [Kofler and Brukner, 2013]. It was defined by the authors as follows: "*No-signaling in time* (NSIT): A measurement does not change the outcome statistics of a later measurement."

Let $p(A_{t_A})$ ($p(B_{t_B})$) be the probability for a variable A (B) measured at time t_A (t_B), and $t_B > t_A$, the NSIT can be mathematically expressed as

$$p(B_{t_B}) = p(B_{t_B|t_A}) \equiv \sum_A p(A_{t_A}, B_{t_B}), \tag{2.85}$$

being

$$\sum_A p(A_{t_A}, B_{t_B}) = \sum_A p(A_{t_A}) p(B_{t_B}|A_{t_A}), \tag{2.86}$$

where $p(B_{t_B}|A_{t_A})$ is the probability for the outcome B at t_B, given the outcome A at t_A, and $p(A_{t_A}, B_{t_B})$ is the joint probability of obtaining A at t_A and B at t_B. An operational formulation for NSIT can be found in Ref. [Clemente and Kofler, 2015]. We will further analyse this condition in the context of the comparison between Bell-type and Leggett-Garg inequalities.

2.2.5 Comparing Bell-type and Leggett-Garg inequalities

We now discuss some fundamental aspects concerning the contrast between Bell-type and Leggett-Garg inequalities.

The first of these aspects is related to Fine's theorem [Fine, 1982, Halliwell, 2014]. According to this theorem, Bell inequalities are necessary and sufficient for local realism. Similarly, one may wonder whether there is a Fine theorem for Leggett-Garg inequalities. In Ref. [Clemente and Kofler, 2016], it is shown that equalities such as the *no-signaling in time condi-*

tion, which we present in the following, are both sufficient and necessary for noninvasiveness. Conversely, the authors conclude that there is no set of inequalities which are sufficient for noninvasiveness. Therefore, it is concluded that the Leggett-Garg inequality is only a necessary condition for noninvasiveness.

Another point which is worth mentioning, considering the contrast between Bell-type and Leggett-Garg inequalities, is related to the so-called *Tsirelson bound* [Budroni and Emary, 2014, Budroni et al., 2013]. The Tsirelson bound is an upper bound for the sum of quantum spatial correlations in Bell-type inequalities [Cirel'son, 1980]. For instance, for the CHSH inequality, given the dichotomic observables A_1, A_2, B_1 and B_2, the Tsirelson bound imposes the upper value of $2\sqrt{2}$ to the sum of *quantum* correlations:

$$\langle A_1 B_1 \rangle + \langle A_1 B_2 \rangle + \langle A_2 B_1 \rangle - \langle A_2 B_2 \rangle \leq 2\sqrt{2}. \tag{2.87}$$

For the derivation of this upper bound, see [Cirel'son, 1980]. Hence, we see that the algebraic bound for the CHSH inequality, which is 4, cannot be attained by considering quantum theory. In this way, the violation of the Tsirelson bound by a Bell inequality would indicate new physics beyond quantum theory [Popescu and Rohrlich, 1994, Budroni and Emary, 2014]. One can naturally consider if this maximum quantum value can be understood from physical principles. Indeed, as indicated in Ref. [Budroni et al., 2013], some principles suggest that, "in a world where maximal correlations are observed, the communication complexity is trivial [Popescu and Rohrlich, 1994], a principle established as information causality is violated [Pawlowski et al., 2009], and there exists no reversible dynamics [Gross et al., 2010]". However, even if there are similarities between the Leggett-Garg inequality and Bell-type inequalities, such as the assumption of a joint probability distribution in their derivation [Markiewicz et al., 2014], Budroni and co-authors have shown that the temporal sum of temporal correlations in the Leggett-Garg inequality can attain its algebraic bound by considering more "general" projective measurements[5] [Budroni and Emary, 2014]. As further discussed by the authors, it is not possible to

[5] This more general projective measurements in Ref. [Budroni and Emary, 2014] are achieved by considering *state-update rules* like the von Neumann's [von Neumann, 1932], which states that a quantum state ρ, when measured, is updated according to the following rule: $\rho \to \sum_k \Pi_{\pm}^{(k)} \rho \Pi_{\pm}^{(k)}$, where $\Pi_{\pm}^{(k)}$ are one-dimensional projectors, and the index $\pm$ indicate their association with those outcomes. This strategy is called "degeneracy-breaking" when compared to Lüders' rule [Lüders, 1951, Lüders, 2006], according to

use these same measurement strategies to violate the Tsirelson for Bell-type inequalities. The saturation of the algebraic bound of Bell-type inequalities is only possible within the context of post-quantum theories [Popescu and Rohrlich, 1994].

2.3 General estimation theory: from classical to quantum theory of parameter estimation

We will introduce here a topic which is independent of quantum theory, the so-called classical theory of parameter estimation. We will then use it to present the formulation of the theory of parameter estimation for quantum systems. The quantum theory of parameter estimation provides the theoretical foundations for the field of *quantum metrology* [Giovannetti et al., 2004, Giovannetti et al., 2011, Giovannetti et al., 2006], allowing one to surpass the classical precision in parameter estimation by using quantum systems. This presentation will be based on L. Davidovich's lectures delivered at the Collège de France [Davidovich, 2016].

Consider the following experiment, sketched in Fig. 2.5: a probe is prepared in a suitable initial state, which is then subjected to a dynamical process. At a given instant $t = t_F$, at which we will call the system's state "final state", a measurement is performed. Finally, one associates an estimation for a parameter θ, $\theta = \theta_{est}(j)$, with each experimental result, j. We will first discuss this experiment within the context of classical physics, then we will consider its description in the context of quantum theory.

As our focus here is on the study of the quality of the estimation of the parameter θ, taking into account the processes described above, it is useful to introduce the following general definitions:

- An estimator is called *unbiased* if the following conditions are satisfied, the average taken over all experimental results and where θ_{true}

which $\rho \to \Pi_{\pm}\rho\Pi_{\pm}$, where we have only two (not necessarily one-dimensional) projectors associated with the $\pm$ outcomes, $\Pi_{\pm}$.

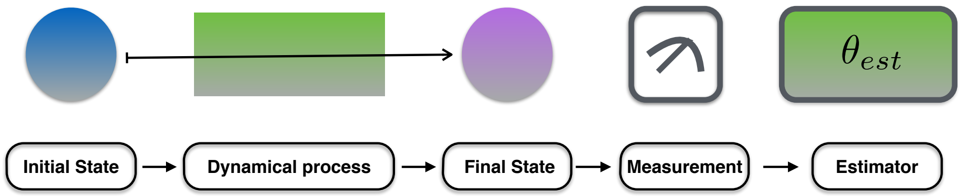

Figure 2.5: Representation of an experiment for estimation of a parameter θ. A probe, prepared in an initial state, is subjected to a dynamical process, leading it to a final state. This final state is then measured, and experimental results j are associated with estimation of the parameter θ. We will discuss this experiment both in the context of classical and quantum theory.

is the true value of the parameter being estimated:

$$\begin{gathered}\langle\theta_{est}\rangle = \theta_{true}, \\ [d\langle\theta_{est}\rangle/d\theta]|_{\theta=\theta_{true}} = 1.\end{gathered} \tag{2.88}$$

- The variance of θ_{est} can be expressed as an average taken over all experimental results as well:

$$\Delta\theta^2 = \left\langle[\theta_{est} - \langle\theta_{est}\rangle]^2\right\rangle. \tag{2.89}$$

2.3.1 Classical parameter estimation

Given an unbiased estimator, the classical lower bound for the variance of θ_{est}, $\Delta\theta$, is determined by the *Cramér-Rao bound* [Fisher, 1912, Cramér, 1946, Rao, 1973]:

$$\Delta\theta \geq \frac{1}{\sqrt{NF(\theta)|_{\theta=\theta_{true}}}}. \tag{2.90}$$

In the equation above, N is the number of experimental realizations and $F(\theta)$ is called *Fisher information*, defined as

$$F(\theta) \equiv \sum_j p_j(\theta) \left(\frac{d \ln p_j(\theta)}{d\theta} \right)^2 , \tag{2.91}$$

where $p_j(\theta)$ are the probabilities of obtaining the result j. Similarly, for a continuous spectrum of measurements results ξ, the Fisher information can be written as

$$F(\theta) \equiv \int d\xi p(\xi|\theta) \left(\frac{\partial \ln p(\xi|\theta)}{\partial\theta} \right)^2 , \tag{2.92}$$

$p(\xi|\theta)$ being the probability distribution of obtaining the result ξ.

Derivation of the Cramér-Rao bound

Consider an unbiased estimator, $\langle \theta_{est}(\xi) \rangle = \theta$, which therefore satisfies the following trivial identity:

$$\int d\xi p(\xi|\theta)[\theta_{est}(\xi) - \theta] = 0. \tag{2.93}$$

By differentiating it with respect to θ, one obtains:

$$\int d\xi \left\{ \frac{\partial p(\xi|\theta)}{\partial\theta} [\theta_{est}(\xi) - \theta] + p(\xi|\theta) \frac{\partial}{\partial\theta} [\theta_{est}(\xi) - \theta] \right\} = 0,$$

or even

$$\int d\xi p(\xi|\theta) \frac{\partial \ln p(\xi|\theta)}{\partial\theta} [\theta_{est}(\xi) - \theta] = 1.$$

We now use the *Cauchy-Schwartz inequality*:

$$\langle A^2 \rangle \langle B^2 \rangle \geq |\langle AB \rangle|^2, \tag{2.94}$$

where

$$
\begin{aligned}
A &= \frac{\partial \ln p(\xi|\theta)}{\partial\theta}, \\
B &= \theta_{est}(\xi) - \theta.
\end{aligned}
\tag{2.95}
$$

In this way, (2.94) reads

$$
\left\langle \left[\frac{\partial \ln p(\xi|\theta)}{\partial\theta} \right]^2 \right\rangle \langle (\Delta\theta_{est})^2 \rangle \geq 1, \tag{2.96}
$$

where $(\Delta\theta_{est})^2 = (\theta_{est} - \langle\theta_{est}\rangle)^2 = (\theta_{est} - \theta)^2$.

Therefore, (2.96) gives:

$$
(\Delta\theta_{est})^2|_{\theta=\theta_{true}} \geq \left[\frac{1}{\left\langle \left[\frac{\partial \ln p(\xi|\theta)}{\partial\theta} \right]^2 \right\rangle} \right]_{\theta=\theta_{true}}. \tag{2.97}
$$

One can then see that the denominator of the expression above is the Fisher information, already defined in the expression (2.91). Alternatively, the Fisher information can be written as follows:

$$
\begin{aligned}
\left\langle \left[\frac{\partial \ln p(\xi|\theta)}{\partial\theta} \right]^2 \right\rangle &= \int d\xi p(\xi|\theta) \left[\frac{\partial \ln p(\xi|\theta)}{\partial\theta} \right]^2 \\
= \int d\xi \frac{1}{p(\xi|\theta)} \left[\frac{\partial p(\xi|\theta)}{\partial\theta} \right]^2 &= -\left\langle \frac{\partial^2 \ln p(\xi|\theta)}{\partial\theta^2} \right\rangle.
\end{aligned}
\tag{2.98}
$$

Finally, given many identical and independent measurements, in such a way that the probability distribution associated with the ensemble of measurements is

$$
p(\vec{\xi}|\theta) = p(\xi_1|\theta)\dots p(\xi_N|\theta), \tag{2.99}
$$

where $p(\xi_i|\theta)$ is the probability of obtaining the result ξ_i, if the value of the parameter is θ. Let $F(\theta)$ be the Fisher information corresponding to a measurement. Therefore, the Fisher information $F^{(N)}(\theta)$, associated with the ensemble of measurements, can be written as:

$$F^{(N)}(\theta) = -\left\langle \frac{\partial^2 \ln p(\vec{\xi}|\theta)}{\partial\theta^2} \right\rangle . \tag{2.100}$$

It follows then that

$$F^{(N)}(\theta) = NF(\theta), \tag{2.101}$$

i. e., the Fisher information fulfils the property of additivity. One can write the Cramér-Rao bound for unbiased estimators as

$$\Delta\theta \geq \frac{1}{\sqrt{NF(\theta)}}, \tag{2.102}$$

where $\Delta\theta \equiv \sqrt{(\Delta\theta_{est})^2}$.

2.3.2 Quantum theory of parameter estimation

We will now discuss the extension of Cramér-Rao-Fisher theory to quantum theory. Therefore, the experiment sketched in Fig. 2.5 is now considered in the context of quantum theory [Helstrom, 1976, Holevo, 1982, Braunstein et al., 1996, Braunstein and Caves, 1994]. Loosely speaking, the precision associated with the determination of the parameter will now depend on the distinguishability between quantum states which are, in turn, associated to nearby values of the parameter.

Quantum Cramér-Rao bound

The derivation of the Cramér-Rao bound is as before. However, the probability distribution of obtaining the result ξ, given that the value of the parameter is θ, and the probe's quantum state $|\psi(\theta)\rangle$, is

$$p(\xi|\theta) = \langle\psi(\theta)\,|\,E(\xi)\,|\,\psi(\theta)\rangle\,, \tag{2.103}$$

where $E(\xi)$ are POVM elements describing a given generalized measurement. Accordingly, the set $\{E(\xi)\}$ satisfies the equations below:

$$\int d\xi E(\xi) = \mathbb{I}, \tag{2.104}$$

so that

$$\int d\xi p(\xi|\theta) = 1. \tag{2.105}$$

In this way, given a set $\{E(\xi)\}$, the lower bound for the estimation of the parameter θ can be written as

$$\sqrt{\langle(\Delta\theta_{est})^2\rangle} \geq \frac{1}{\sqrt{NF(\theta)}}, \tag{2.106}$$

where the Fisher information $F(\theta)$ can be expressed as

$$F(\theta;\{E(\xi)\}) = \int d\xi p(\xi|\theta)\left[\frac{\partial \ln p(\xi|\theta)}{\partial\theta}\right]^2 = \int d\xi \frac{1}{p(\xi|\theta)}\left[\frac{\partial p(\xi|\theta)}{\partial\theta}\right]^2. \tag{2.107}$$

One can note that equation 2.107 corresponds to a specified quantum measurement, described by a given set $\{E(\xi)\}$. One may therefore pose the question of what would be the best possible estimation, which would be correspondently associated with a particular measurement. The best possible estimation is in turn associated with the ultimate lower bound for $\langle(\Delta\theta_{est})^2\rangle$, for which the Fisher information is maximal. In this particular case, the Fisher information is called *quantum Fisher information*, and can be obtained through an optimization of the Fisher information over all quantum measurements specified by each set $\{E(\xi)\}$. This can be written as in the following expression:

$$\mathcal{F}_Q = \max_{\{E(\xi)\}} F(\theta, \{E(\xi)\}), \tag{2.108}$$

so that the improved variance now reads

$$\langle(\Delta\theta_{est})^2\rangle \geq \frac{1}{N\mathcal{F}_Q}. \tag{2.109}$$

As before, N is the number of experimental realizations.

Quantum Fisher information for pure states

In the following, we derive the expression of the quantum Fisher information for pure states. As, we will see that it can be simply expressed as the variance of the system's Hamiltonian.

Let us consider a unitary process $U(\theta)$, and the initial state of a probe, $|\psi(0)\rangle$. As illustrated in Fig. 2.5, the final θ-dependent state is

$$|\psi(\theta)\rangle = U(\theta)\,|\psi(0)\rangle\,. \tag{2.110}$$

Before proceeding, it will be useful to define an auxiliary operator $\hat{h}$

$$\hat{h}(\theta) = -i\frac{dU(\theta)}{d\theta}U^{\dagger}(\theta). \tag{2.111}$$

Using the definition of $\hat{h}$, one can write:

$$\begin{aligned}\frac{d\,|\psi(\theta)\rangle}{d\theta} = \frac{dU(\theta)}{d\theta}\,|\psi(0)\rangle &= \frac{dU(\theta)}{d\theta}U^{\dagger}(\theta)\,|\psi(\theta)\rangle \\ &= i\hat{h}(\theta)\,|\psi(\theta)\rangle\,.\end{aligned} \tag{2.112}$$

One can therefore see that the equation above is equivalent to the Schrödinger equation with Hamiltonian $-\hat{h}(\theta)$. The operator $-\hat{h}(\theta)$ is then called the *generator* of $U(\theta)$.

We now recall equations (2.103) and (2.104). Considering them, one can derive the following equation:

$$\begin{aligned}\frac{\partial p(\xi|\theta)}{\partial\theta} &= \left[\frac{d\,\langle\Psi(\theta)|}{d\theta}\right]E(\xi)\,|\Psi(\theta)\rangle + \langle\Psi(\theta)|\,E(\xi)\left[\frac{d\,|\Psi(\theta)\rangle}{d\theta}\right] \\ &= i\,\langle\psi(\theta)|\,[E(\xi),\hat{h}]\,|\psi(\theta)\rangle = -2\Im[\langle\psi(\theta)|\,E(\xi)\hat{h}(\theta)\,|\psi(\theta)\rangle]\end{aligned} \tag{2.113}$$

One can alternatively write the equation above considering a real function $g(\theta)$, as

$$\frac{\partial p(\xi|\theta)}{\partial\theta} = -2\Im[\langle\psi(\theta)|\,E(\xi)[\hat{h}(\theta)-g(\theta)]\,|\psi(\theta)\rangle]. \tag{2.114}$$

By squaring the expression above, we are able to obtain the following result

$$\begin{aligned}\left[\frac{\partial p(\xi|\theta)}{\partial\theta}\right]^2 &= 4[\Im[\langle\psi(\theta)|\, E(\xi)[\hat{h}(\theta)-g(\theta)]\,|\psi(\theta)\rangle]]^2 \\ &\le 4|\,\langle\psi(\theta)|\, E^{1/2}(\xi)E^{1/2}(\xi)[\hat{h}(\theta)-g(\theta)]\,|\psi(\theta)\rangle\,|^2 \\ &\le 4\,\langle\psi(\theta)\,|\,E(\xi)\,|\,\psi(\theta)\rangle\,\langle\psi(\theta)|\,E(\xi)[\hat{h}(\theta)-g(\theta)]^2\,|\psi(\theta)\rangle\,,\end{aligned} \tag{2.115}$$

where, in the last step, we used the Cauchy-Schwartz inequality (2.94). In this way, we obtain the expression below:

$$\left[\frac{\partial p(\xi|\theta)}{\partial\theta}\right]^2 \le 4p(\xi|\theta)\,\langle\psi(\theta)|\,E(\xi)[\hat{h}(\theta)-g(\theta)]^2\,|\psi(\theta)\rangle\,. \tag{2.116}$$

Finally, dividing the expression above by $p(\xi|\theta)$ and integrating it with respect to ξ, we have

$$\begin{aligned}F(\theta) = \int d\xi\frac{1}{p(\xi|\theta)}\left[\frac{\partial p(\xi|\theta)}{\partial\theta}\right]^2 &\le 4\int d\xi\,\langle\psi(\theta)|\,E(\xi)[\hat{h}(\theta)-g(\theta)]^2\,|\psi(\theta)\rangle \\ &= 4\,\langle\psi(\theta)|\,[\hat{h}(\theta)-g(\theta)]^2\,|\psi(\theta)\rangle\,,\end{aligned} \tag{2.117}$$

given that $\int d\xi E(\xi) = 1$.

One can therefore see that the Fisher information $F(\theta)$ is upper-bounded by the quantity $4\,\langle\psi(\theta)|\,[\hat{h}(\theta)-g(\theta)]^2\,|\psi(\theta)\rangle$. We now rewrite the expression above in terms of the initial state $|\psi(0)\rangle$:

$$F(\theta) \le 4\,\langle\psi(0)|\,[\hat{H}(\theta)-g(\theta)]^2\,|\psi(0)\rangle\,, \tag{2.118}$$

where

$$\hat{H}(\theta) \equiv U^\dagger(\theta)\hat{h}(\theta)U(\theta) = -iU^\dagger(\theta)\frac{dU(\theta)}{d\theta}. \tag{2.119}$$

Specifically, by employing the following expression of $U(\theta)$,

$$U(\theta) = \exp(i\theta\hat{O}), \tag{2.120}$$

where $\hat{O}$ is independent of θ, it results then that $\hat{H}(\theta) = \hat{O}$. One can note that, if $\hat{O}$ is a Hamiltonian, θ is consequently a time displacement, $U(\theta)$ being the evolution operator. We can then see that the minimum value for the bound is attained when

$$g(\theta) = \left\langle \psi(0) \middle| \hat{H}(\theta) \middle| \psi(0) \right\rangle \equiv \langle \hat{H}(\theta) \rangle_0. \tag{2.121}$$

Then, we are finally able to write the following expression for the upper-bound of the Fisher information:

$$F(\theta) \leq 4 \langle (\Delta \hat{H})^2 \rangle_0, \tag{2.122}$$

with

$$\langle (\Delta \hat{H})^2 \rangle_0 \equiv \langle \psi(0) | \, [\hat{H}(\theta) - \langle \hat{H}(\theta) \rangle_0]^2 \, | \psi(0) \rangle \, . \tag{2.123}$$

Hence, we have shown that, for pure states, the upper bound for the Fisher information, called *quantum Fisher information*, is given by

$$\mathcal{F}_Q = 4 \langle (\Delta \hat{H})^2 \rangle_0. \tag{2.124}$$

Alternatively, by using the definition of $\hat{H}$, the quantum Fisher information for pure states can be also written as follows:

$$\mathcal{F}_Q = 4 \left[\frac{d \langle \psi(\theta) |}{d\theta} \frac{d | \psi(\theta) \rangle}{d\theta} - | \, \frac{d \langle \psi(\theta) |}{d\theta} | \psi(\theta) \rangle \, | \right]. \tag{2.125}$$

For pedagogical purposes, we will show in the following how this ultimate lower bound can be obtained analytically for pure states, leading to a simple expression for the quantum Fisher information.

When the Fisher information equals the quantum Fisher information: pure state case

Consider the state $|\psi(\theta')\rangle$, and the measurement defined by

$$\begin{aligned} E_1 &= |\psi(\theta)\rangle \langle \psi(\theta)| \, , \\ E_2 &= 1 - |\psi(\theta)\rangle \langle \psi(\theta)| \, . \end{aligned} \tag{2.126}$$

We show here that the Fisher information corresponding to this measurement attains the quantum Fisher information when $\theta' \to \theta$. For the measurement defined above, the probability p_1 and p_2 of obtaining the result 1 and 2, respectively, are:

$$\begin{aligned} p_1(\theta') &= \mid \langle \psi(\theta') \mid \psi(\theta') \rangle \mid^2 \\ p_2(\theta') &= 1 - p_1(\theta'). \end{aligned} \tag{2.127}$$

It follows then that the corresponding Fisher information is:

$$\begin{aligned} F_\theta(\theta') &= \frac{1}{p_1(\theta')} \left[\frac{dp_1(\theta')}{d\theta'} \right]^2 + \frac{1}{p_2(\theta')} \left[\frac{dp_2(\theta')}{d\theta'} \right]^2 \\ &= \frac{1}{p_1(\theta')[1 - p_1(\theta')]} \left[\frac{dp_1(\theta')}{d\theta'} \right]^2 . \end{aligned} \tag{2.128}$$

Now, given that $\lim_{\theta' \to \theta} p_1(\theta') = 1$ and $\lim_{\theta' \to \theta} \left[\frac{dp_1(\theta')}{d\theta'} \right] = 0$, it results that the limit $\theta' \to \theta$ of the Fisher information is indeterminate. Therefore, by applying l'Hôpital's rule, one obtains

$$\lim_{\theta' \to \theta} F_\theta(\theta') = -2 \left[\frac{d^2 p_1(\theta')}{d\theta'^2} \right] = 4 \left\langle \psi(0) \,\middle|\, (\Delta \hat{H})^2 \,\middle|\, \psi(0) \right\rangle . \tag{2.129}$$

where, as defined before, $\hat{H} \equiv i \frac{dU^\dagger(\theta)}{d\theta} U(\theta)$.

One can then see that this is precisely the upper bound found before, *i. e.*, the quantum Fisher information for pure states.

2.3.3 General expression for the Fisher information and quantum Fisher information

The expression of the Fisher information can be generalized by noting that the derivative of the probability can be written in a symmetrical form [Luo, 2004]:

$$\frac{\partial p(\theta)}{\partial \theta} = \frac{1}{2} \left(\frac{\partial}{\partial \theta} (\ln p(\theta)).p(\theta) + p(\theta).\frac{\partial}{\partial \theta} (\ln p(\theta)) \right) \tag{2.130}$$

In Equation (2.92), we replace the integration by trace, and the parametrized probability $p(\theta)$ by a corresponding density operator

$$\rho_\theta = e^{-i\theta\hat{H}}\rho_0 e^{i\theta\hat{H}}, \tag{2.131}$$

where ρ_0 is the initial state in Fig. 2.5, and ρ_θ, the evolved or final state. Also, we replace the logarithmic derivative by the *symmetric logarithmic derivative*, L_θ, determined by

$$\frac{\partial}{\partial\theta}\rho_\theta = \frac{1}{2}(L_\theta\rho_\theta + \rho_\theta L_\theta). \tag{2.132}$$

In so doing, by using (2.130) and (2.132), we can express the quantum Fisher information $\mathcal{F}_Q(\rho_\theta)$ as

$$\mathcal{F}_Q(\rho_\theta) = Tr(L_\theta^2\rho_\theta). \tag{2.133}$$

This expression is quite useful and allows one to calculate the quantum Fisher information of a given quantum state ρ_θ.

By using the general expression for the quantum Fisher information given by (2.133), one can easily show that the quantum Fisher information does not depend on the parameter θ. This is a consequence of the cyclic property of the trace:

$$\begin{aligned}\mathcal{F}_Q &= Tr(\rho_\theta L_\theta^2) = Tr(e^{-i\theta\hat{H}}\rho_0 e^{i\theta\hat{H}}L_\theta^2)\\ &= Tr(\rho_0 e^{-i\theta\hat{H}}L_\theta^2 e^{i\theta\hat{H}}).\end{aligned} \tag{2.134}$$

By using the fact that ρ_θ satisfies the von Neumann-Liouville equation,

$$i\frac{\partial\rho_\theta}{\partial\theta} = H\rho_\theta - \rho_\theta H, \tag{2.135}$$

and considering also equation (2.132), we have

$$i(\rho_\theta H - H\rho_\theta) = \frac{1}{2}(L_\theta\rho_\theta - \rho_\theta L_\theta). \tag{2.136}$$

This last equation implies the following one

$$i(\rho_0 H - H\rho_0) = \frac{1}{2}(L\rho_0 - \rho_0 L), \tag{2.137}$$

with $L = e^{-i\theta H} L_\theta e^{i\theta H}$.

We can see that L is independent of θ, as H and ρ_0 in (2.137), are also independent of θ. In this way, one can show that the quantum Fisher information is independent of the parameter θ, since, as a result of (2.134), we have

$$\mathcal{F}_Q = Tr(\rho_0 L^2). \tag{2.138}$$

Chapter 3

Modeling Leggett-Garg inequality violation

As we have seen in the previous chapter, the Leggett-Garg inequality is a test of the nonclassicality of a system, and involves correlations between measurements performed at different times. According to its original interpretation, a violation of the Legget-Garg inequality disproves macroscopic realism and noninvasiveness. Nevertheless, macroscopic realism is a model dependent notion, and one should always be able to attribute to measurement invasiveness a violation of a Legget-Garg inequality. Given this, we introduce, in the present chapter, an operational model where the effects of invasiveness are controllable through a parameter associated with what is called the measurability of the physical system. Such a parameter leads to different generalized measurements that can be associated with the dimensionality of a system, measurement errors, or back action. This work has been published as an article in Phys. Rev. A [Moreira et al., 2015].

3.1 Introduction

In the previous chapter, we gave an overview of quantum theory and highlighted some of its contrasts with our everyday-based intuition. One may wonder if what is at the heart of the quantum mechanical incoherences with our world is the elusive definition of what is "classical". Indeed, one may be tempted to define as classical everything that does not seem to behave quantum mechanically, as for instance objects on the human scale. Nevertheless, this definition is not very helpful, since it is not more straightforward to define what one means by "behave quantum mechanically" than it is to do the opposite.

One aspect of quantum theory that is incompatible with classical theory, defined as local and realist by Einstein, Podolsky and Rosen [Einstein et al., 1935, Bohr, 1935], is Bell-type inequality violations [Bell, 1964, Clauser et al., 1969, Aspect et al., 1982b]. However, one cannot safely assert that all states that do not violate these inequalities are classical. Perhaps, as suggested by our presentation in the previous chapter, the most general property of quantum mechanics is contextuality [Cabello, 2008, Cabello et al., 2015, Kochen and Specker, 1967], which can be observed for *any* quantum state [Cabello, 2008, Badziag et al., 2009]. Assuming noncontextuality allows one to derive inequalities, of which Bell's are a special case. Such inequalities suffer, in their broader and state independent version, from a lack of intuitive interpretation. They do not classify quantum states according to any usefulness they may have as a resource, or any of their particular properties that would help one's understanding of the quantum-classical frontier.

With this goal in mind, in the 1980s, Leggett and Garg [Leggett and Garg, 1985] proposed an inequality which is often presented as enabling us to witness nonclassicality of a (macroscopic) system when violated. We recall briefly the expression and discussion of the Leggett-Garg inequality which we introduced in the previous chapter. The Leggett-Garg inequality involves measurements of a two-valued quantity Q at different times, defined here as $Q(t_i)$. By defining $C_{kl} \equiv \langle Q(t_k)Q(t_l)\rangle$, the Leggett-Garg inequality can be written as:

$$-2 \leq K_{LG} \equiv C_{12} + C_{23} + C_{34} - C_{14} \leq 2. \tag{3.1}$$

As formerly introduced by Leggett and Garg and presented before in this thesis, the Leggett-Garg inequality must be satisfied if the assumptions of (macroscopic) realism and noninvasive measurability hold. Thus, the Leggett-Garg inequality violation would imply nonclassicality by the terms of both assumptions.

Notwithstanding, there has been a lively debate in the recent literature about the interpretation of the Leggett-Garg inequality violation [O. J. E. Maroney, 2014, Clemente and Kofler, 2015, Clemente and Kofler, 2016, Moreira et al., 2016]. According to what we have seen before, Maroney and Timpson [O. J. E. Maroney, 2014] have shown that Leggett and Garg's first assumption, namely macroscopic realism, is model-dependent. In the authors point of view, as usually interpreted in the Leggett-Garg inequality, this assumption is analogous to a superselection rule [Zurek, 2003] that prepares the system in a statistical mixture of some privileged states. According to this definition, violating the Leggett-Garg inequality would imply that the system is, at some point during its evolution, in a quantum superposition. However, the notion of quantum superposition is not necessarily incompatible with either macroscopicity or with realism, and depends on the specific interpretation of quantum theory considered. For instance, as discussed in chapter 2, if the Bohm-de Broglie's interpretation [Bohm and Hiley, 1993] is taken into account, then the meaning of the violation of the Leggett-Garg inequality can be put in question [O. J. E. Maroney, 2014]. It is then concluded that the only notion that can actually be tested in a model-independent way by the Leggett-Garg inequality is measurement invasiveness.

It is also worth mentioning that the notion of macroscopicity in the Leggett-Garg inequality has always been somewhat controversial. Indeed, since one of the mathematical requirements in the derivation of the Leggett-Garg inequality is that correlations between measurements should be correlations between dichotomic observables, one may wonder what is the sense of macroscopicity. Can one speak of macroscopicity when only two effective numbers are assigned to each observable?

Therefore, before proceeding, we first discuss how the notion of macroscopicity lacks of a general definition and depends on the conditions of the experiment considered.

3.1.1 "Micro. versus Macro."

We have previously seen in chapter 2 that assumption *(i)* can be generally called realism instead of macrorealism. The notion of realism applies to physical systems irrespective of their size, and the use of the prefix "macro" in "macrorealism" would express our intuition that macroscopic objects are supposed to have a classical description. However, to my knowledge, we still do not dispose of a general definition of macroscopicity. One may wonder, indeed, if such a more general definition is possible.

Macrorealist theories are required to provide the regimes in which quantum theory ceases to be valid, *i. e.* the *level* or *scale* at which quantum theory applies [Knee, 2014]. A possible way of studying the quantum-to-classical frontier is to apply the Leggett program [Takagi, 2005,Knee, 2014], which consists of testing the Leggett-Garg inequality considering physical systems of progressively increased sizes.

This is illustrated in Fig. 3.1, taken from [Knee, 2014], where the blue polygon delimits the region of validity of quantum theory on the parameter space specified by the set of parameters $\{r_i\}$, which can be defined, for instance, as the number of particles, mass, distance etc. On the other hand, if it is verified experimentally that quantum theory is valid in a region of parameter space delimited by the set of parameters $\{s_i\}$, as illustrated by the red polygon of Fig. 3.1, then one is able to establish the failure of a macrorealist description in that region of the parameter space.

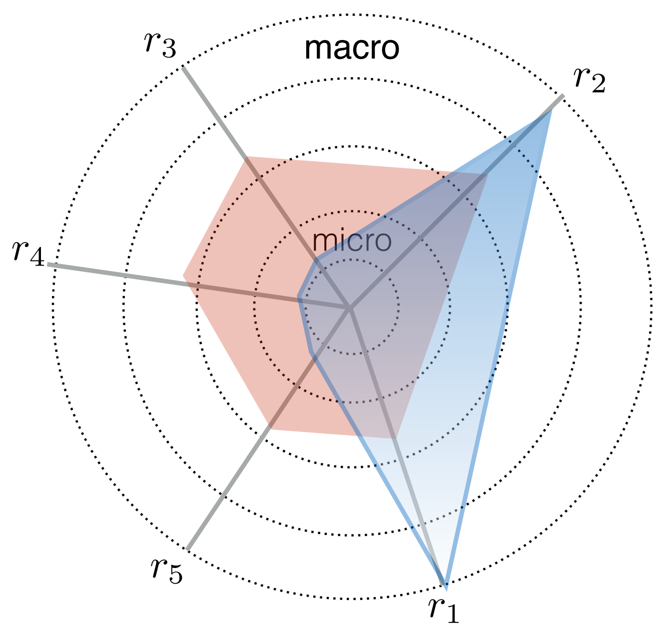

Figure 3.1: Illustration shown in Ref. [Knee, 2014], where the blue polygon represents the region of validity of quantum theory imposed by macrorealism theories, for instance. The region in red represents experimental data which can violate macrorealism for a set of parameters which are larger than is fixed by the theory of macrorealism in question. The different parameters r_i can be the number of particles, mass, etc.

In Ref. [Kofler and Brukner, 2007], of which results are discussed in detail below, some physical insight was provided to help to interpret the role of a specific aspect of macroscopicity in the Leggett-Garg inequality, defined as the limit of $j \to \infty$. Within this model, measurements become coarse-grained or noisier in this limit and, consequently, noninvasive. It is this specific definition of macroscopicity which we consider whenever we refer to this term in the present chapter.

3.1.2 Is there any relationship between invasiveness and macroscopicity?

The more general approach mentioned above, wherein the Leggett-Garg inequality primarily tests measurement invasiveness, becomes even clearer if one considers the mathematical formulation of the Leggett-Garg inequality. Indeed, this formulation makes explicit what features of correlations between measurement results are being tested.

To this end, one should consider that observables $Q(t_i)$ are measured, in each of the many runs of an experiment, in order to compute the statistical average needed to obtain the correlations C_{kl}. As we have seen in details in the previous chapter, when the two-time correlations C_{kl} are computed in the situation where the four measurements $Q(t_i)$ $(i = 1, 2, 3, 4)$ were realized, inequality (3.1) is always satisfied, both in the classical and in the quantum realm. The relevant experimental realizations are those when one considers the case where only the two measurements $Q(t_k)$ and $Q(t_l)$ are made in each run to compute C_{kl}. In this case, Eq. (3.1) is valid only if the noninvasiveness assumption is made. This last situation (two measurements at each run) corresponds to the Leggett-Garg inequality.

Thus, a possible reformulation of what is tested by a Leggett-Garg inequality would be:

> *The Leggett-Garg inequality tests the pertinence of the hypotheses that correlations between two-measurement outcomes realized at different times are undisturbed by the realization of other measurements to the system at different times.*

Given this formulation, how can one understand previous works, where macroscopicity seemed to enhance coarse-graining or noise, being at the origin of a quantum-to-classical transition? Is it possible to model and control measurement invasiveness in a way that does not depend on the system's size? We aim to provide answers to these questions in the following sections of this chapter. Before addressing them, we will introduce the aforementioned model, due to Kofler and Brukner, in which macroscopicity is associated to coarse graining.

3.2 Kofler and Brukner's model

In this section and in the remainder of this chapter, we will consider a spin-j system [Cohen-Tannoudji et al., 1973]. Spin-j systems can be associated, *e.g.*, with an atom or an orbital angular momentum.

Let J_α, $\alpha = x, y, z$, be the α-component of $\mathbf{J}$, the total spin operator. Eigenstates of the operator j_z are denoted as $|m\rangle$, $-j \leq m \leq j$. It will be considered that the dynamics of the system is governed by the Hamiltonian:

$$H = \Omega \mathbf{J}^2 + \omega J_x, \tag{3.2}$$

where Ω and ω are constants with the dimension of frequency.

We will now review the results of Ref. [Kofler and Brukner, 2007], which uses a spin-j system as described above. In this study, Kofler and Brukner have shown that classical physics can arise out of quantum mechanics by increasing the size of a system, more specifically, in the limit of infinitely large j. In order to demonstrate this, the authors first consider the special case of a spin-j *coherent state*.

Spin-j coherent states are defined as the eigenstates $|\theta, \phi\rangle$ with maximal eigenvalue of the total spin operator $\mathbf{J}$ pointing in the direction (θ, ϕ)[1], where θ and ϕ are the polar and azimutal angles respectively, *i. e.*,

$$\mathbf{J} |\theta, \phi\rangle = j |\theta, \phi\rangle .$$

Let $|\theta_0, \phi_0\rangle$ be the initial state at $t = 0$, where (θ_0, ϕ_0) define the direction in which the total spin $\mathbf{J}$ operator is initially pointing, be given by the following expression:

$$|\theta_0, \phi_0\rangle = \sum_m \binom{2j}{j+m}^{1/2} \cos^{j+m} \frac{\theta_0}{2} \sin^{j-m} \frac{\theta_0}{2} e^{-im\phi_0} |m\rangle . \tag{3.3}$$

This initial state will evolve in time according to the Hamiltonian of (4.15), such that the evolution operator is given by $U(t) = e^{-iHt}$. This unitary corresponds therefore to a rotation over the yz-plane.

[1] Alternatively, one may define spin-j coherent states in the following way: starting from $J_z |j, j\rangle = j |j, j\rangle$, and defining $|\theta, \phi\rangle := D^j(R_{\theta,\phi}) |j, j\rangle$, where $R_{\theta,\phi}$ represents the rotation from the vertical axis to the direction (θ, ϕ), we have $D^j(R_{\theta,\phi}) J_z D^j(R_{\theta,\phi})^\dagger |\theta, \phi\rangle = j |\theta, \phi\rangle$.

By taking into consideration this initial state and evolution, the probability that a J_z measurement gives the outcome m at time t is

$$p(m,t) = |\langle m\,|\,\theta,\phi\rangle|^2,$$

with $\cos\theta = \sin\omega t \sin\theta_0 \sin\phi_0 + \cos\omega t \cos\theta_0$, θ and ϕ being the polar and azimutal angle of the rotated spin coherent state $|\theta,\phi\rangle$ at time t.

If now one considers the limit $j \gg 1$ it then shown that the expression for the probability distribution can be approximated by a Gaussian distribution

$$p(m,t) \approx \frac{1}{\sqrt{2\pi}\sigma} e^{-(m-\mu)^2/2\sigma^2}, \tag{3.4}$$

with a width given by $\sigma \equiv \sqrt{j/2}\sin\theta$ and $\mu \equiv j\cos\theta$.

Let us now define "slots" of finite size Δm, which subdivide the $2j+1$ possible outcomes into a smaller number $\frac{2j+1}{\Delta m}$ of slots. The size of the slot, Δm, is defined as the resolution of the *measurement apparatus*. Now, consider that in the limit of infinite dimensionality, $j \to \infty$, Δm scales slower than j, $\Delta m = o(j)$, and that the relation $\Delta m \gg \sqrt{j}$ is always satisfied. As illustrated by Fig. 3.2, it follows then that in such conditions, the slot will become infinitely narrow. In this manner, the Gaussian distribution (3.4) will tend to the Dirac delta function:

$$p(m,t) \to \delta(m-\mu). \tag{3.5}$$

Then, it is possible to show that an entirely classical description of the system is valid in such a limit. This classical description can be put in terms of a *spin vector* $\mathbf{J}$ (length $J \equiv |\mathbf{J}| = \sqrt{J(J+1)} \approx J$, when $J \gg 1$) which at $t=0$ points in the (θ_0,ϕ_0)-direction, and which evolves in time according to the Hamilton function

$$H = \Omega\mathbf{J}^2 + \omega J_x. \tag{3.6}$$

At any time, the probability that the z-component of the spin vector, $J\cos\theta$, is in slot m is given by $\delta(m-\mu)$ (3.5), as if the time evolution of the spin components J_α ($\alpha = x,y,z$) were described by the classical Hamilton equations of motion

$$\dot{J} = [J_\alpha, H]_{PB}. \tag{3.7}$$

According to (3.6), the solutions correspond to a rotation around the x-axis. Put differently, in the proper continuum limit, the spin vector at

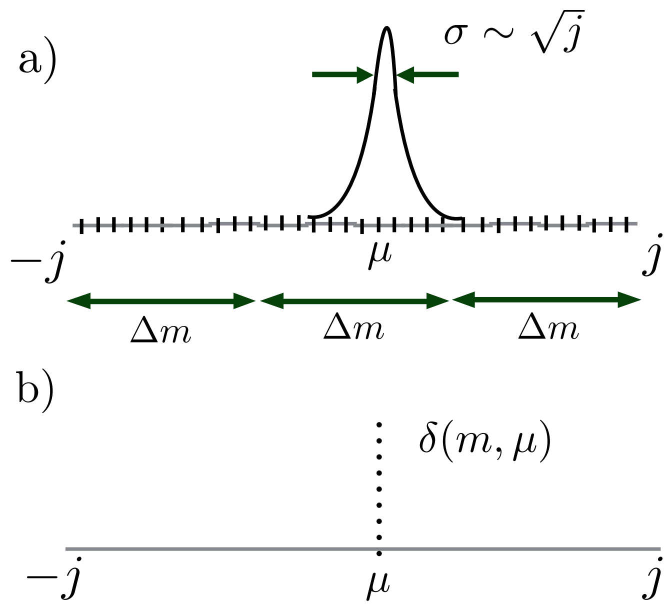

Figure 3.2: a) Representation of the probability distribution $p(m, t)$ that an outcome m is obtained when measuring a spin coherent state at time t for $j \ll 1$ (3.4). b) As $j \to \infty$ and $\Delta m = o(j)$, $p(m, t)$ becomes infinitely narrow, tending to the Dirac delta function $\delta(m - \mu)$.

time t points in the (θ, ϕ)-direction where θ and ϕ correspond to those of the spin-j coherent state, and the prediction is given by $\delta(m-\mu)$. One can then note that this corresponds to a classical description of a spin vector. Measurements are therefore not invasive within this classical description.

The authors go further by showing a generalization of the result described above for arbitrary spin-j states, which we will not reproduce here. See Ref. [Kofler and Brukner, 2007] for the details.

To conclude, this result illustrates how a dimension-dependent coarse-graining allows us to retrieve a classical description as $j \to \infty$.

3.3 Modeling measurement invasiveness in the Leggett-Garg inequality

With the purpose of formalizing the discussion of the previous sections and determining in a precise mathematical way the interplay between invasiveness, dimensionality and violation of the Leggett-Garg inequality, we propose a model to test the Leggett-Garg inequality using positive operator valued measure (POVM).

As we will see, invasiveness can be associated with the resolution and efficiency of a measurement apparatus within this model. Depending on the experimental situation, these parameters may or may not be associated with the dimensionality of the system. In this way, the introduced POVMs provide a physically sound and operational interpretation of what is actually being tested by the Leggett-Garg inequality, providing a clarification of the relationship between the notions of invasiveness and macroscopicity.

In what follows, we will consider spin-j systems, such as those described in the previous section. We start by defining the initial state, and then introducing generalized measurements. These measurements are defined by parameters which, in principle, can be controlled in the experiment.

The initial state is defined as a maximally mixed state,

$$\rho(0) \equiv \frac{1}{2j+1} \sum_{m=-j}^{j} |m\rangle \langle m| \,. \tag{3.8}$$

This choice of initial state is motivated by the fact that it ensures that non-classicality can only appear from the system's dynamics and the subsequent measurements.

In Ref. [Kofler and Brukner, 2007], it was shown that measurements defined by the observable $\hat{Q}(0) = \hat{\Pi}_z$, where

$$\hat{\Pi}_z = \sum_m (-1)^{j-m} |m\rangle \langle m| \,, \tag{3.9}$$

is the parity operator, lead to violation of a Leggett-Garg inequality irrespectively of the dimensionality of the system, for a maximally mixed initial state of the J_z eigenstates (3.8).

Indeed, projective parity measurements involve all the states $|m\rangle$, which creates the analogous of "collective states" associated with a single quantum number. Therefore, it reduces systems of any dimension to an effective two level system through a mapping that applies to all possible states: the time evolution of the parity operator involves all the system's states in the same way (except for a sign change). It is thus intuitively acceptable that such a measurement will always lead to a Leggett-Garg inequality violation, since one can hardly think of a less invasive dichotomic measurement. Based on this fact, our approach consists in defining an observable depending on a parameter σ that, at one of its extremal values, corresponds to the parity operator.

We then write the binary correlations C_{kl} as follows:

$$C_{kl} \equiv p_+^{kl} q_{+|+}^{kl} + p_-^{kl} q_{-|-}^{kl} - p_+^{kl} q_{-|+}^{kl} - p_-^{kl} q_{+|-}^{kl}. \tag{3.10}$$

where $p_\pm^{kl}$ are the probabilities of measuring one of the outcomes ± 1, and $q_{\pm|\pm}^{kl}$ are the probabilities of obtaining the $\pm$ outcomes conditioned to those which were previously obtained. This property of the binary correlations C_{kl} were already explored in a recent work by Asadian *et al.*, where a Leggett-Garg inequality test using the measurement of periodic observables defined in an nanomechanical oscillator is proposed [Asadian et al., 2014]. In [Ketterer et al., 2015] it is shown that Bell-type inequalities can be performed using observables with an arbitrary spectrum. In both works, the key ingredient is the definition of a two-valued POVM $\hat{M}_\pm$, as follows:

$$\hat{E}_\pm = \hat{M}_\pm^\dagger \hat{M}_\pm = \frac{1}{2}(1 \pm \hat{A}), \tag{3.11}$$

where $\hat{A}$ is an operator with a spectrum in the interval $[-1, 1]$.

It is known, in light of Neumark's theorem introduced in chapter 2, that each element of the above defined POVM, identified by the signs $\pm$, is associated with one of the two possible outcomes (± 1) of a projective measurement realized in an auxiliary two dimensional Hilbert space. Thus, operators $\hat{A}$ have a spectrum bounded between ± 1, since

$$\begin{gathered} \langle \hat{A} \rangle = P_+ - P_-, \text{ and} \\ P_+ + P_- = 1, \end{gathered} \tag{3.12}$$

where $P_\pm$ are the probabilities of obtaining one of the two possible outcomes of measurements realized in the aforementioned auxiliary two dimensional space.

3.3.1 The model

We now introduce the expression of the operator $\hat{A}$, which satisfies all the above mentioned properties:

$$\hat{A} \equiv \sum_{\mu} \sum_{m \in \Delta m_{\mu}} (-1)^{(j-m)} f_{\mu}(m,\sigma) \left|m\right\rangle \left\langle m\right| , \tag{3.13}$$

where $f_{\mu}(m,\sigma) = e^{\frac{-(m-\mu)^2}{2\sigma^2}}$ and Δm_{μ} are disjoint sets containing equally sized intervals of m. All these parameters in the expression of $\hat{A}$ are illustrated in Figs. 3.4 and 3.5. In the following discussion, we interpret and discuss them.

First of all, one can see that the operator (3.13) allows the description of both perfect and imperfect parity measurements. For instance, if $f_{\mu}(m,\sigma) = 1\ \forall m$, $\hat{A}$ becomes the parity operator, and $\hat{E}_{\pm}$ are perfect, projective measurements. In this case, to each m is assigned a ± 1 eigenvalue, according to the parity of $j - m$. Otherwise, this operator describes an imperfect parity measurement, as we will see below. Indeed, this interpretation will be completed by providing a physical meaning for the parameters σ, μ and Δm_{μ}. These parameters will be associated with the concepts of *measurability*, *optimal measurement*, and *measurement resolution*, respectively.

We start by interpreting Δm_{μ}, the measurement resolution. It determines the number of eigenvalues N, among all the possible values of m, that the measurement apparatus can faithfully detect. Faithfully detecting means here detecting and assigning the correct value of m to a particle. Each of these perfectly determined values is defined as the optimal measurement μ. In this way, the total number of different values $m = \mu$ is given by

$$N = \frac{(2j+1)}{\mathcal{N}(\Delta m_{\mu})}, \tag{3.14}$$

where $\mathcal{N}(\Delta m_{\mu})$ is the number of elements in Δm_{μ}.

We provide an illustration of these concepts within the context of a Stern-Gerlach type experiment. In this way one can see, with the help of Fig. 3.3, that $m = \mu$ corresponds to a perfect Stern-Gerlach type measurement: the z-axis projection of the spin with value $m = \mu$ is deflected by an angle $\theta_m = \theta_{\mu}$ that allows one to identify the position it hits on the screen, and associate it to the correct value of m univocally. In view of (3.13), this can be translated in the following way: for $m = \mu$, $f_{\mu}(m,\sigma) = 1$ irrespectively of the value of σ. A correct and well defined parity is therefore associated with these values of m, *i. e.*,

$$\langle \hat{A} \rangle_{m=\mu} = (-1)^{(j-m)} = \langle \hat{\Pi}_z \rangle_{m=\mu} = \pm 1. \tag{3.15}$$

The measurement resolution Δm_μ also defines the interval of values of m that are considered around each μ: each interval Δm_μ defines the domain of a function $f_\mu(m, \sigma)$.

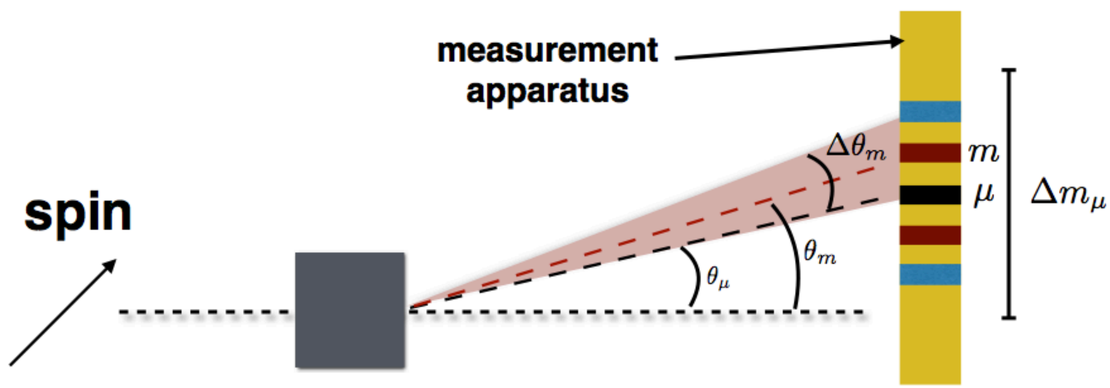

Figure 3.3: Illustration, in the context of a Stern-Gerlach type experiment, of the introduced parameters governing the two valued POVM in Eq. (3.13): a spin-j is deflected by a magnetic field with spatial inhomogeneities. As a consequence, for some values of m ($m = \mu$), the perfect measurement of m is possible (perfect correlation between m and the deflection angle, θ_μ, and the position on the screen, the measurement apparatus). For $m \neq \mu$, uncertainties $\Delta\theta_m$ around the deflection angle θ_m lead to uncertainties in the position of the spin in the measurement apparatus, and consequently, in the value of m. The interval Δm_μ is the resolution of the measurement, in the sense that it determines the number of μ's that can be faithfully measured (*i. e.*, are associated to a fixed position in the screen).

Finally, we define the parameter σ, the *measurability*. Later, we will see that it can be related to measurement invasiveness. This parameter is a measure of the *unfaithfulness* of the measurement. By unfaithfulness, we mean the following scenario: for finite σ and $m \neq \mu$, the particle is detected, but the value of m cannot be perfectly determined. Thus, it will be sometimes associated with the correct value, or to a value with the same parity (and then the correct parity will be assigned to it) and sometimes associated with a value of m corresponding to a different parity. As a consequence, for $m \neq \mu$, one cannot assign a well-defined parity, and, as a consequence, we have

$$\langle \hat{A} \rangle_{m\neq\mu} = (-1)^{(j-m)} e^{\frac{-(m-\mu)^2}{2\sigma^2}}. \tag{3.16}$$

Note that, in particular, for σ such as $f_\mu(\mu+1,\sigma) = 0$, $\langle \hat{A} \rangle_{m\neq\mu} = 0$ and $\langle \hat{E}_\pm \rangle = 1/2$, we have the equivalent of a perfectly random parity measurement. Physically, unfaithfulness of measurements could arise, in the context of a Stern-Gerlach type experiment, as a consequence of position dependent fluctuations of the magnetic field, which can create an uncertainty $\Delta\theta_m$ in the deflection angle depending on the value of m. All these parameters are illustrated in Fig. 3.4, where we plotted $g \equiv f_\mu(m,\sigma)$, with $\mathcal{N}(\Delta m_\mu) = 3$ and $\sigma = 0.6$.

We conclude this discussion by noting that the limit of $\sigma \to \infty$ (perfect measurability) is equivalent to that of perfect resolution ($f_\mu(m,\sigma) = 1 \forall m$, $\mathcal{N}(\Delta m_\mu) = 1$), since all the values of m are associated to a μ, and $N = 2j+1$.

In what follows, we will move to an example which illustrates how the introduced parameters can control measurement invasiveness in a way that is dimension independent. We then discuss how the aforementioned parameters can be modified, depending on the experimental situation, by the system's dimensionality or measurement efficiency. To this effect, we first notice that the probabilities appearing in (3.10) can be written, for a given pair of measurement times t_k, t_l, as:

$$\begin{aligned} p_\pm^{kl} &= \mathrm{Tr}[E_\pm \hat{\rho}(t_l)], \\ q_{\pm|\pm}^{kl} &= \mathrm{Tr}[E_\pm \hat{\rho}_\pm(t_k)], \end{aligned} \tag{3.17}$$

where we have used (3.2), with $\hat{U}(t_k - t_l) = e^{-i\theta_{kl}\hat{J}_x}$, with $\theta_{kl} = \omega(t_k - t_l)$. In (3.17), $\rho_\pm(t_k)$ is the state of the system just before the second measurement, performed at time t_k. The index $\pm$ correspond to the two possible outputs obtained just after the first measurement which have been performed at time t_l ($t_l < t_k$). Therefore, the state at time t_k, just before the second measurement, is given by

$$\hat{\rho}_\pm(t_l) = \hat{U}(t_k - t_l)\hat{\rho}_\pm(t_k)\hat{U}^\dagger(t_k - t_l) = e^{-i\theta_{kl}\hat{J}_x}\hat{\rho}_\pm(t_k)e^{i\theta_{kl}\hat{J}_x}, \tag{3.18}$$

with

$$\hat{\rho}_\pm(t_k) = \frac{\hat{M}_\pm \hat{\rho}(t_k)\hat{M}_\pm^\dagger}{p_\pm} = \frac{1 \pm \hat{A}}{2(2j+1)p_\pm}. \tag{3.19}$$

The probabilities $q_{+|\pm}$ can be therefore expressed as:

$$q_{+|\pm} = \frac{1}{2p_\pm}\mathrm{Tr}\left[\left(\frac{1+\hat{A}}{2}e^{-i\theta_{kl}\hat{J}_x}\left(\frac{1\pm\hat{A}}{2j+1}\right)\right)e^{i\theta_{kl}\hat{J}_x}\right]. \tag{3.20}$$

Then, it turns out that the correlations C_{kl} are given by

$$C_{kl} = \frac{1}{(2j+1)}\mathrm{Tr}(\hat{A}e^{i\theta_{kl}\hat{J}_x}\hat{A}e^{-i\theta_{kl}\hat{J}_x}). \tag{3.21}$$

Now, it is known that for an arbitrarily given value for j, the general expansion formula for the evolution operator is [**?**]

$$e^{i\phi(\vec{n}.\vec{j})} = \sum_{r=0}^{2j}\frac{c_r(\phi)}{r!}(2i\hat{\mathbf{n}}.\mathbf{J}\sin(\phi/2))^r, \tag{3.22}$$

where $\hat{\mathbf{n}}$ is an arbitrary unitary vector, ϕ is the rotation angle around $\hat{\mathbf{n}}$ and the coefficients $c_r(\phi)$ are such that

$$c_r(\phi) = (\cos(\phi/2))^\epsilon \mathrm{Trunc}_{[j-r/2]}\left(\frac{(\arcsin\sqrt{x}/\sqrt{x})^r}{(\sqrt{1-x})^\epsilon}\right), \tag{3.23}$$

where $x = \sin^2(\phi/2)$ and $\epsilon(j-r/2) = \frac{1-(-1)^{2j-r}}{2}$.

It turns out, then, that by using this expansion, one can evaluate the correlations of (3.21).

3.3.2 An example: spin $5/2$

We illustrate the model by considering an example with $j = 5/2$ (a six-level system). In order to be able to identify the parameters introduced above, we will only consider two possible values of μ, $\mu_\pm = \pm 5/2$, and $\Delta m_{\mu_\pm} = [\pm 5/2, 0]$ (intersection between the two sets is unimportant, since 0 is not a possible value of m).

In this simple example, we can identify three possible values of $f_{\mu_\pm}(m,\sigma)$, namely a, b and c, obeying the following relations: $a = 1$ (for $m = \pm 5/2$) and $c = b^4$ (for $m = \pm 1/2$), with $b = e^{-1/2\sigma^2}$ (for $m = \pm 3/2$), since the $f_{\mu_\pm}(m,\sigma)$ considered here is a Gaussian distribution centered at $\mu_\pm$.

It is clear that modifying σ leads to a modification of b and c only (a is constant, as previously defined). Thus, for $\sigma \ll 1$, only $\mu_\pm = \pm 5/2$

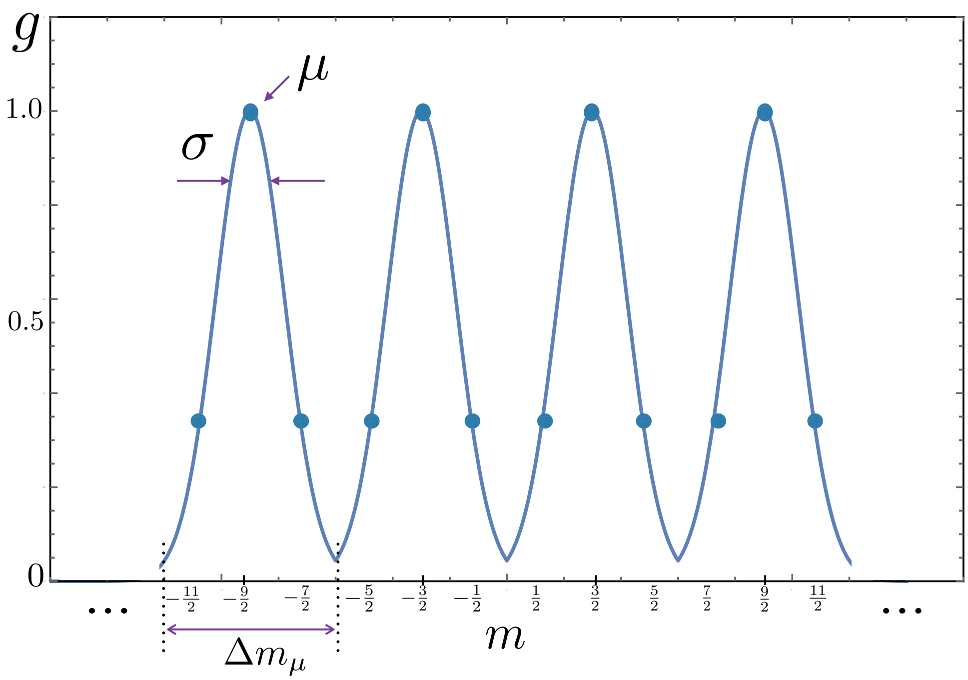

Figure 3.4: Representation of the function g and definition of the parameters of the POVM in Eq. (3.13) as a function of m: the measurement results μ are the central values of m in the interval Δm_μ. For $m = \mu$, $g = 1$. The width σ determining the measurability is associated to the width of the Gaussian function defined in each interval Δm_μ. Nevertheless, we can see that it is not the usual variance, since irrespective of its value, $g = 1$ for $m = \mu$. In the Figure, $\sigma = 0.6$ and the number of elements in Δm_μ is given by $\mathcal{N}(\Delta m_\mu) = 3$.

are faithfully measured while for $\sigma \to \infty$ the operator $\hat{A}$ tends to a parity measurement.

We computed K_{LG} as a function of b (which here, equivalently to σ, is related to the measurability) and of time. We considered, for simplifying and illustrative reasons, only measurement times such as $k = l + 1$ and define $\theta_{l+1l} \equiv \theta$. Results are plotted in Fig. 3.6. One can notice that the absolute value of K_{LG} increases monotonically with b for the cases where the inequality is violated for some b. Nonetheless, its maximum is always reached for $b = 1$, which corresponds to $\sigma \to \infty$. In this situation, we retrieve the parity operator $\hat{\Pi}_z$, and we have perfect measurability and measurement resolution.

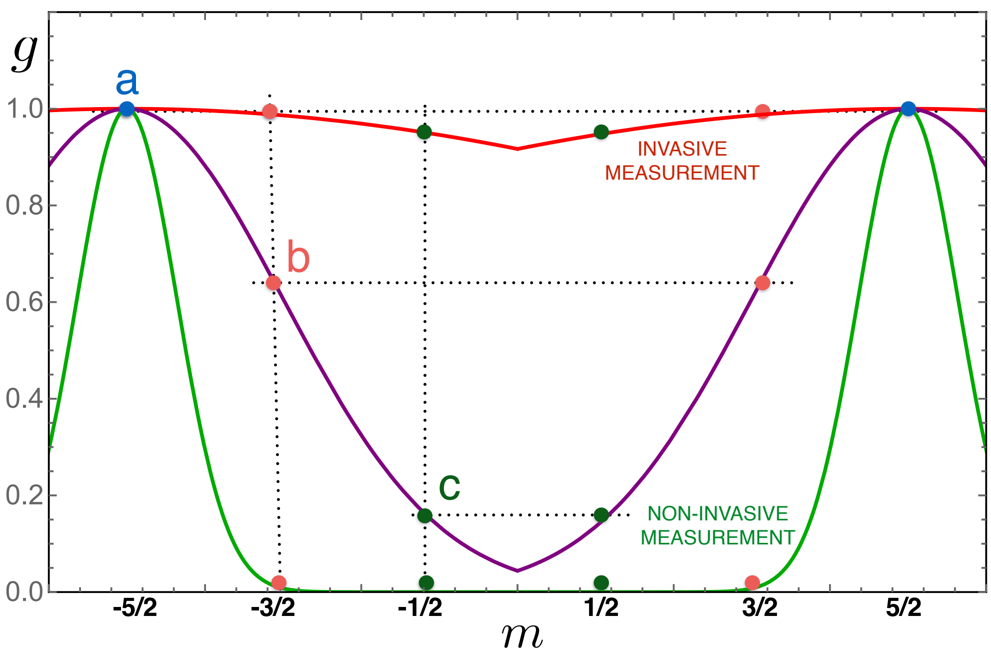

Figure 3.5: Representation of the three possible values of g (a, b and c) in the illustrative case of $j = 5/2$ as a function of σ for the case where $m_\pm = \pm 5/2$ are optimally measured. The parameters a, b and c are represented for three possible choices of b (and consequently c): red, $b = 0.98$ is associated to a invasiveness measurement, and high measurability; purple, $b = 0.61$ and green, $b = 0.008$ are associated to non invasiveness measurements (from up to bottom curve, respectively).

We can thus associate invasiveness to measurability: the more a system is measurable, in the sense that the more one can faithfully detect different values of m (higher value of b), the more the Leggett-Garg inequality is violated.

Measurability is a dimension independent definition, but it can perfectly well depend on the dimensionality of a system in a similar way as in Ref. [Kofler and Brukner, 2007]. By making Δm_μ increase faster with j than σ, one can, by increasing j, lose violation of the Leggett-Garg inequality. In the present measurement model, this can be understood easily as an increase of the measurability that is slower than the increase in resolution (increase of σ slower than of Δm_μ). Nevertheless, such a behavior can be observed irrespective of the dimension of the system.

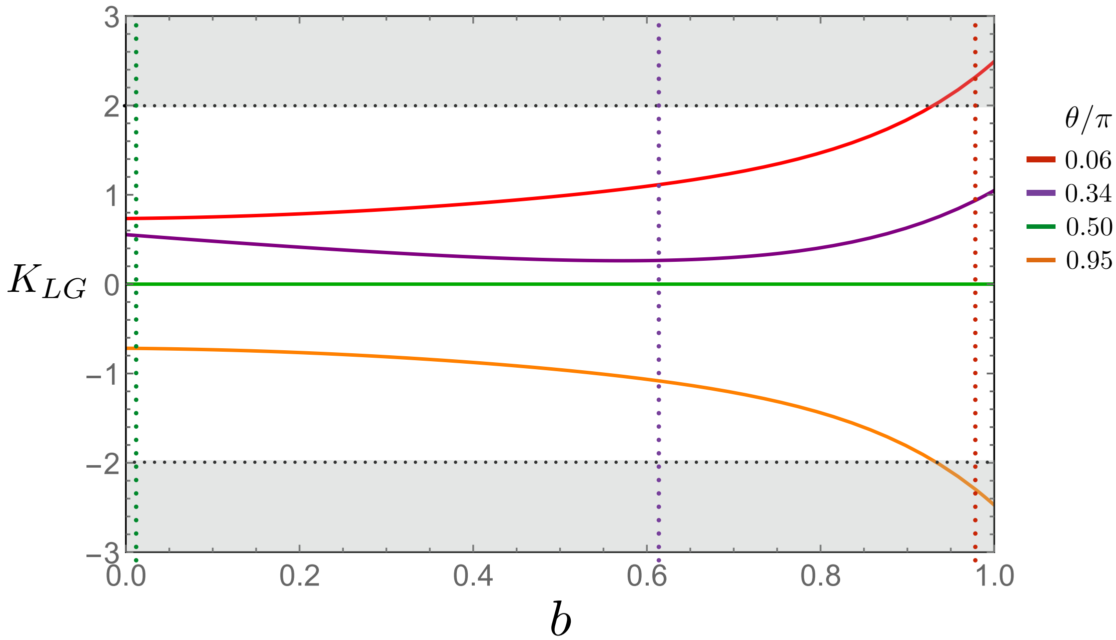

Figure 3.6: Legget-Garg parameter, K_{LG} (Eq. (3.1)) as a function of b for the following values of θ/π (from up to bottom curve, respectively): 0.06 (red), 0.34 (purple), 0.50 (green), 0.95 (orange). We identified, for the cases where violation is observed for some value of b (red and orange curves, corresponding to 0.06 and 0.95 as values for θ/π, respectively) the values of b corresponding to the functions g plotted in Fig. 3.5. They are represented by dotted vertical lines: red for $b = 0.98$, purple for $b = 0.61$ and green for $b = 0.008$. The chosen color code is the same as in Fig. 3.5.

Finally, one should note that the proposed model can also be interpreted as a measure of disturbance of a measurement: unfaithful measurements can also be modeled by a measurement that highly disturbs the system, *i. e.*, modifies the value of m during the measurement process. Consequently, a value of m is assigned to a state but, after the measurement process, it is no longer applicable. In this context, our model easily connects the introduced parameters to the notion of classical back action and disturbance of a measurement. The more classical back action is introduced, the less the Leggett-Garg inequality is violated, which would exclude the possibility of the clumsiness loophole [Wilde and Mizel, 2012], described in detail in chapter 4.

3.4 Conclusion

To conclude, we provided a toy model where the violation of the Leggett-Garg inequality can be directly controlled and understood through physically sound parameters. These parameters can be associated with the unfaithfulness of a measurement, a notion that can have different physical origins, all of them contemplated in the introduced model. One example is the increase of dimensionality of the system and another one is the classical disturbance created by the measurement process.

While each parameter's precise interpretation depends on the physical system one uses to test a Leggett-Garg inequality, the role of each parameter is clearly identified and related to the invasiveness, whatever its physical origin is. Thus, this notion is shown to be, operationally, the most fundamental one that is tested in a Leggett-Garg inequality. Our model can be used to help understanding and interpretation of Leggett-Garg inequality tests, and can be tested experimentally in a number of physical systems, such as Stern-Gerlach-like experiments with inhomogeneous fields, or the orbital angular momentum of photons.

Chapter 4

Connecting measurement invasiveness to optimal metrological scenarios

The connection between the Leggett-Garg inequality and optimal scenarios from the point of view of quantum metrology is investigated for perfect and noisy general dichotomic measurements. In this context, we show that the Fisher information can be expressed in terms of quantum temporal correlations. This connection eventually allows us to associate scenarios with relatively high Fisher information to scenarios in which the Leggett-Garg inequality is violated, which leads therefore to a connection between measurement invasiveness and more or less favorable metrological scenarios. Finally, we illustrate our results by using a model for spin systems.

4.1 Introduction

As mentioned in the previous chapter, the term "macroscopic" has always been intuitively associated with classical physics. *Macroscopic objects*, for instance, are the ones observed in our everyday life scale, and are expected to behave classically. It is known that classical physics fails to provide a description of phenomena at the microscopic level, which demand the application of quantum mechanical principles, such as the superposition principle and entanglement. Therefore, one is naturally led to the question of whether such quantum mechanical principles could also be observed at the macroscopic scale. This fundamental question concerning the validity of extrapolating quantum mechanics to the macroscopic world [Leggett, 2002] was already pictured in 1935 in the Schrödinger's cat *Gedanken* experiment [Schrödinger, 1935], where superpositions of states ("dead" and "alive") of a macroscopic object (the cat) are at stake.

In chapter 3, we introduced an operational model relating the Leggett-Garg inequality violation with a parameter called the *measurability* of physical systems. We illustrated our results using perfect and noisy parity measurements performed in spin-j systems. According to our model, the more the system is "measurable", *i.e.*, the more one is able to faithfully distinguish between its different possible outcomes, the more the Leggett-Garg inequality is violated. Maximum measurability therefore corresponds to projective measurements. As measurability decreases and the measurements become weaker, Leggett-Garg inequality violation progressively ceases, vanishing at some point. Therefore, measurability is clearly associated with the invasiveness of measurements, which in turn can depend *e.g.* on measurement errors or on a dimension-dependent coarse graining [Kofler and Brukner, 2007]. According to this model, the violation of the Leggett-Garg inequality does not intrinsically depend on the system's size, a notion that lacks itself of precise definition whenever quantum systems are concerned [Yadin and Vedral, 2016, Fröwis et al., 2016, Kwon et al., 2016].

Recently, remarkable experimental achievements and experimental proposals regarding Leggett-Garg inequality violation for systems which can be reasonably considered macroscopic, in relation to a given parameter, were presented in Refs. [Knee et al., 2012, Formaggio et al., 2016, Budroni et al., 2015].

4.1.1 A connection between temporal correlations and quantum metrology?

Seemingly unconnected, the field of quantum metrology has recently attracted considerable attention [Giovannetti et al., 2004, Giovannetti et al., 2011, Giovannetti et al., 2006, Paris, 2009, Escher et al., 2011a, Escher et al., 2011b, Alipour et al., 2014, Fröwis et al., 2016, Mehboudi et al., 2016, Braun et al., 2017]. The use of some quantum mechanical states as probes for the sake of estimating a parameter θ has been shown to lead to a better scaling, with the dimension of the state, of the precision in the parameter's estimation than using classical resources only. For noisy systems, it was shown that this scaling actually depends on the system's size, the noise parameter and noise model [Escher et al., 2011a]. Ultimately, for a fixed dimension of the probe state, the precision of the estimation of θ usually decreases as the noise parameter increases, unless one resorts to appropriate control or error-correcting methods [Braun et al., 2017].

In light of these elements, it thus seems natural to investigate connections between the Leggett-Garg violation and quantum metrology. In the present chapter, we investigate connections between temporal correlations, and ultimately the Leggett-Garg inequality violation, and quantum metrology. As we will see later, we will do so by identifying each step of the Leggett-Garg inequality test with the steps of a metrological scenario.

Hence, before proceeding, it will be useful to recall the context of parameter estimation theory [Fisher, 1912, Cramér, 1946, Rao, 1973], which we have discussed in details in chapter 2.

The definition of classical Fisher information (called, from now on, Fisher information) is as follows: consider a parameter θ, the value of which will be estimated through the measurement of a given observable. It is clear that, if the result of the measurement is independent of θ, then no information about this parameter can be obtained. Conversely, if the output of the measurement is very sensitive to the value of θ, the measurement will allow us to infer a more accurate value of θ. The Fisher information is a way to characterize this sensitivity of the measurement of a given observable to the estimation of the value of the parameter θ. Assuming unbiased measurements (implying that the average of the estimated value over all experimental results coincides with the true value of the parameter), the standard deviation $\Delta\theta$ can be written as

$$\Delta\theta \geq \frac{1}{\sqrt{\nu F}}, \tag{4.1}$$

where ν is the number of repetitions of the experiment. For a given measurement, F is given by

$$F(\theta) = \sum_l P_l(\theta) \left[\frac{\partial \ln P_l(\theta)}{\partial\theta}\right]^2, \tag{4.2}$$

where the $P_l(\theta)$ are the probabilities of obtaining each one of the different outcomes l, satisfying $\sum_l P_l(\theta) = 1$. The generalization of the Fisher information to quantum mechanics is done by writing $P_l(\theta) = \mathrm{Tr}[\rho(\theta)E_l]$, where E_l is a *positive operator valued measure* (POVM). By maximizing $F(\theta)$ over all quantum measurements, one obtains the quantum Fisher information (QFI) $\mathcal{F}_Q$ [Helstrom, 1976, Holevo, 1982, Braunstein et al., 1996, Braunstein and Caves, 1994], associated with the minimum lower bound for $\Delta\theta$, and saturated when $\nu \to \infty$. The quantum Fisher information provides an upper bound to the Fisher information, and corresponds therefore to the Fisher information associated with the optimal measurement, *i.e.* the one which gives the best estimation for θ.

4.2 Leggett-Garg inequality and metrological protocols

4.2.1 The correlation function

In this section, we compare the Leggett-Garg inequality test scenario to a parameter estimation protocol and establish some general results. In a Leggett-Garg inequality test, an initially maximally mixed state

$$\rho_0 = \frac{\mathbb{I}}{d},$$

is prepared, where d is the dimension of the underlying Hilbert space.

We denote by $\hat{A}$ the dichotomic observable measured in the Leggett-Garg inequality, and $U(t_i) = e^{-iHt_i}$ the unitary time evolution, generated by the Hamiltonian H. From now on, we suppose that, by rescaling the energies, the times t_i are dimensionless.

Using these definitions, we have seen in chapter 3 that the two-time correlation appearing in (3.1) can be written as

$$C_{kl} = \mathrm{Tr}[\hat{A}U(t_k - t_l)\hat{A}U(t_k)\rho_0 U^\dagger(t_k)U_j^\dagger(t_k - t_l)] = C(\theta_{kl}), \tag{4.3}$$

where $\theta_{ij} \equiv t_i - t_j$.

We can then define the *correlation function* $C(\theta)$ as follows,

$$C(\theta) = \frac{1}{d}\mathrm{Tr}[\hat{A}\hat{U}(\theta)\hat{A}\hat{U}^\dagger(\theta)], \tag{4.4}$$

where all the time intervals $\theta = t_2 - t_1 = t_3 - t_2 = t_4 - t_3$ are the same. The correlation functions C_{kl} in the Leggett-Garg inequality (3.1) are called *stationary* if they depend only the time difference θ [Emary et al., 2014]. Under this consideration, the Leggett-Garg inequality

$$-2 \leq K_{LG} \equiv C_{12} + C_{23} + C_{34} - C_{14} \leq 2, \tag{4.5}$$

can be rewritten as

$$|K_{LG}| = |3C(\theta) - C(3\theta)| \leq 2. \tag{4.6}$$

Before proceeding, let us discuss Eq. (4.6). Generally, in a Leggett-Garg test as described by (4.5), one must perform four independent experiments in order to measure each one of the correlations C_{12}, C_{23}, C_{34} and C_{14}. As we assumed that the time intervals $\theta = t_2 - t_1 = t_3 - t_2 = t_4 - t_3$ are the same, it suffices to determine only two terms: $C(\theta)$ and $C(3\theta)$. Therefore, only two independent experiments, in which one performs two subsequent measurements, are required in this case. In this way, one can therefore notice that K_{LG} (or C) can be expressed as a function of θ, the time difference between subsequent measurements.

Since we consider a maximally mixed state as initial state, the system's state will remain the same before the first measurement for any unitary transformation. After the first measurement, however, the system's state will be one of the two possible outcomes resulting from the measurement of $\hat{A}$. We shall thus refer to the first measurement as the *preparation procedure.*

4.2.2 A parallel between the metrological scenario and Leggett-Garg's

We introduce here a metrological scenario which will be related to the Leggett-Garg inequality protocol described above. We consider the problem of estimating the parameter θ through the measurement of the dichotomic observable $\hat{A}$. This measurement, as in the case of a Leggett-Garg inequality test, can correspond either to ideal, projective or to noisy measurements, and can be generally described by a two-valued POVM. Such measurements will be performed on a probe state, and will play a crucial role on the ultimate precision that can be reached for the estimation of θ.

In order to establish a parallel between a metrological protocol and the Leggett-Garg inequality we will consider the probe state to be one of the possible outcomes of the preparation procedure, *i.e.*, the state prepared as result of the first measurement. Because we consider a maximally mixed initial state, the results of the first measurement of $\hat{A}$ are equally probable. That is, each one of the two possible states associated with the preparation procedure can be obtained with equal probabilities 1/2. As we will see below in the derivation of the expression of the Fisher information, these two states give the same results for an estimation of θ.

The quality of the estimation of the parameter θ is characterized by the Fisher information $F(\theta)$ given by Eq. 4.2, in which $P_l(\theta)$, with $l = \pm 1$, is the probability for measuring each one of the two elements of the dichotomic observable $\hat{A}$.

In this way, following the preparation procedure, at the time the second measurement is performed, the evolved system's state read

$$\rho_+(\theta) = U(\theta)\rho_+ U^\dagger(\theta), \tag{4.7}$$

if the system's state is ρ_+, *i.e.* as a result of recording the outcome "+1" at the time of the first measurement. Similarly, the evolved state will read

$$\rho_-(\theta) = U(\theta)\rho_- U^\dagger(\theta), \tag{4.8}$$

if the system's state is ρ_-, *i.e.* if the outcome"−1" is obtained at the first measurement.

It follows then that the Fisher information $F(\theta)$ of either $\rho_+(\theta)$ or $\rho_-(\theta)$ can be expressed as a function of the correlation function $C(\theta)$ as

$$F(\theta) = \frac{1}{1 - C(\theta)^2}\left[\frac{\partial C(\theta)}{\partial \theta}\right]^2. \tag{4.9}$$

Derivation of (4.9)

In the following, we will show that Eq. (4.9) can be derived by considering either $\rho_+(\theta)$ or $\rho_-(\theta)$ as the preparation state. Explicitly, we can express the two-valued POVMs as

$$\hat{E}_\pm = \hat{M}_\pm^\dagger \hat{M}_\pm = \frac{1}{2}(1 \pm \hat{A}). \tag{4.10}$$

In this way, if $\rho_+(\theta)$ is considered, the probabilities of obtaining the outcomes $\pm$ at the time at which of the second measurement is performed can be written as

$$p_\pm(\theta) = \mathrm{Tr}(\hat{E}_\pm \rho_+(\theta)) = \frac{1}{2} \pm \frac{1}{2}C(\theta), \tag{4.11}$$

if $\rho_+(\theta)$ is considered as the preparation state, and

$$p_\pm(\theta) = \mathrm{Tr}(\hat{E}_\pm \rho_-(\theta)) = \frac{1}{2} \mp \frac{1}{2} C(\theta), \tag{4.12}$$

if one considers the preparation $\rho_-(\theta)$ instead.

Finally, one obtains Eq. (4.9) by considering either the probability distribution (4.11) or (4.12) in Eq. (4.2).

Hence, in (4.9) we have the expression of the Fisher information as a function of quantum temporal correlations. This expression has, therefore, several remarkable properties and will serve as guideline to establish a connection between the Leggett-Garg inequality and the Fisher information. As we will see, it will allow us to introduce the nonclassical notion of measurement invasiveness in the context of metrological processes, and discuss how it is associated with (nearly-)optimal scenarios for parameter estimation. Before this, however, we will first discuss Eq. (4.9).

4.2.3 Connecting the Fisher information to temporal correlations

In (4.9), we first note that the extrema of $C(\theta)$ (for which $\frac{\partial C}{\partial \theta} = 0$) are also extrema of $F(\theta)$. This follows from the derivation of (4.9):

$$\frac{\partial F}{\partial \theta} = \frac{1}{(1 - C^2)^2} \left[2(1 - C^2) \frac{\partial C}{\partial \theta} \frac{\partial^2 C}{\partial \theta^2} + 2C \left(\frac{\partial C}{\partial \theta} \right)^2 \right]. \tag{4.13}$$

A priori, the extrema of $C(\theta)$ are not all extrema of $F(\theta)$, but let us focus on their common extrema, which we will label by θ_e.

It is straightforward to show that θ_e is a maximum of F if and only if $C(\theta_e)^2 = 1$. The value $C = \pm 1$ can only be obtained for an ideal projective measurement. In particular, if we have such an extremum of C at $\theta = 0$, and if $C(\theta)$ is a periodic function with period denoted by T (which is the case if the Bohr frequencies of H are commensurate), then $\theta = nT$ ($n \in \mathbb{N}$) will also correspond to extrema. In this last case, as $C(\theta)$ is an even function, *i.e.* it fulfills the condition $C(\theta) = C(-\theta)$, it can be shown that $\theta = nT/2$ is also an extremum of $C(\theta)$. The global extremum correspond to the value $C(nT/2)^2 = 1$ only for ideal projective measurements.

On the other hand, if an extremum of C is such that $C(\theta_e)^2 \neq 1$, then $F(\theta_e) = 0$ and θ_e is necessarily a minimum of F. This is the case for noisy measurements.

Therefore, we find a very peculiar situation, in which the estimation of θ_e can be optimal when the measurement is ideally projective but all information about θ_e is lost when an infinitesimal amount of noise is added to the measurement. Indeed, if the noise is such that

$$C(\theta_e) = 1 - \epsilon, \tag{4.14}$$

then $F(\theta_e) = 0$, for ϵ as small as one wishes. In other words, the maximum of F which is also an extremum of C is not robust against noisy measurements for parameter estimation.

4.3 Parity measurement on a spin system

The expression of the Fisher information as a function of $C(\theta)$ (4.9) is quite general, and is only based on the fact that dichotomic measurements are performed in the experiment described by the protocol presented above for parameter estimation. In the following, we will consider a specific example which illustrates its consequences.

We will study the case of parity measurements performed in a spin-j system. Parity was shown to be useful in quantum optical metrology [Chiruvelli and Lee, 2011, Gerry and Mimih, 2010], and has also been used in our model, presented in the previous chapter, within which Leggett-Garg inequality violation is controlled through a parameter determining the invasiveness of a POVM.

Let us consider, then, the same system as described in the previous chapter: a spin operator J, with spatial components J_v, $v = x, y, z$. The J_z eigenstates are denoted as $|m\rangle$, $-j \leq m \leq j$, where $j(j+1)$ $(j \in \mathbb{N})$ are the eigenvalues of J^2. The dynamics of the system is governed by the following Hamiltonian:

$$H = \Omega \mathbf{J}^2 + \omega J_x, \tag{4.15}$$

where Ω and ω are constants with the dimension of frequency ($\hbar = 1$). The initial state is given by a maximally mixed state:

$$\rho_0 = \frac{1}{2j+1} \sum_{m=-j}^{j} |m\rangle \langle m| \, , \tag{4.16}$$

in such a way that, within this model, Leggett-Garg inequality violations can only arise from the measurements and system's dynamics. We consider the two-valued POVM in Eq. (4.10) with

$$\hat{A} \equiv \sum_{\mu} \sum_{m \in \Delta m_\mu} (-1)^{(j-m)} f_\mu(m,\sigma) \left|m\right\rangle \left\langle m\right| . \tag{4.17}$$

The functions $f_\mu(m,\sigma) = e^{\frac{-(m-\mu)^2}{2\sigma^2}}$ and Δm_μ are disjoint sets containing equally sized intervals of m. The parameter σ can be interpreted as being associated with the unfaithfulness of the measurement: for finite σ and $m \neq \mu$, the particle is detected, but the value of m cannot be perfectly determined. Hence, $\sigma \to \infty$ implies performing projective measurements, with perfect determination of the system's parity as, for this case, $\hat{A} = \hat{\Pi}_z = \sum_m (-1)^{j-m} \left|m\right\rangle \left\langle m\right|$. Finally, the parameter Δm_μ determines the number N, among all the possible values of m that the measurement apparatus can faithfully detect, and therefore is called the *measurement resolution* of the measurement apparatus.

As the preceding chapter, we study the example of a spin 5/2, which will allow us to illustrate our results. In this example, we introduce a parameter, b, that is directly associated with the measurability of the system, or alternatively, to the invasiveness of a measurement and the width σ of the function $f_\mu(m,\sigma) = e^{\frac{-(m-\mu)^2}{2\sigma^2}}$. As we considered in the previous chapter, by defining $b \equiv e^{-1/2\sigma^2}$, we have that $\sigma \to \infty$ corresponds to $b \to 1$, and $\sigma \to 0$ to $b \to 0$. In (4.17), we consider only two possible values of μ, $\mu_\pm = \pm 5/2$, and the two corresponding intervals are $\Delta m_{\mu_\pm} = [\pm 5/2, 0]$.

We move on to the computation of the Fisher information and the quantum Fisher information relative to the estimation of the parameter θ. As mentioned before, the first parity measurement of the Leggett-Garg inequality is identified as the state preparation procedure in the protocol for parameter estimation. Therefore, this preparation state is one of the following ones:

$$\rho_\pm(t_k) = \frac{(\hat{E}_\pm)^{\frac{1}{2}} \rho_0 (\hat{E}_\pm)^{\frac{1}{2}}}{p_\pm}. \tag{4.18}$$

In the protocol for parameter estimation, we will consider that the state which is prepared as a result of the first measurement is $\hat{\rho}_+$. As we mentioned above, this choice is justified by the fact that either $\hat{\rho}_+$ or $\hat{\rho}_-$ lead to the same results.

By taking into consideration the state's dynamics given by (4.15), the evolved state $\rho_+(\theta)$, immediatelly before the realization of the parity measurement, can be written as follows:

$$\rho_+(\theta) = U(\theta)\rho_+(t_k)U^\dagger(\theta) = e^{-i\theta J_x}\rho_+(t_k)e^{i\theta J_x}. \tag{4.19}$$

Using this state, we computed the Fisher information $F(b, \theta)$ defined by (4.2), corresponding to measurements with the two-valued POVMs given by (4.10). We also evaluated the quantum Fisher information $\mathcal{F}_Q(b)$ by using the expression in Ref. [Liu et al., 2014].

In the following, we split the analysis of the results into two cases: for noise-free parity ($b = 1$) measurements and noisy parity measurements ($b \neq 1$).

4.3.1 Projective parity measurements ($b = 1$)

The results for $b = 1$, *i.e.* for projective, noise-free parity measurements, are shown in Fig. 4.1(a). The Fisher information $F(1, \theta)$ and the quantum Fisher information $\mathcal{F}_Q(b = 1)$ are both shown in this figure.

We see that both quantities are equal for $\theta = n\pi$, showing that the measurement scenario is optimal at this point. We also note that these maxima of $F(1, \theta)$ are also extremum of $C(\theta)$, and, as expected, the correlation function reaches its optimal value $C = \pm 1$ at these points.

We then compare these results to K_{LG} defined in Eq. (2.2) as a function of θ. The point of maximal correlation cannot be a point of Leggett-Garg inequality violation, and this is well illustrated in Fig. 4.1(a). Therefore, invasiveness cannot be witnessed for $\theta = n\pi$. As it is shown in Fig. 4.1(a), the region around $\theta = n\pi$ corresponds to relatively high Fisher information, and maximum Leggett-Garg inequality violation also occurs in this region. In the framework of this model, we see that favorable metrological scenarios occurs in the same region where invasiveness is witnessed through Leggett-Garg inequality violation. Nevertheless, the maximum of the Fisher information does not coincide with the maximum violation of the Leggett-Garg inequality. But as we have seen in the previous section, we expect these maxima of the Fisher information not to be robust against infinitesimal addition of noise to the measurement process.

4.3.2 Noisy parity measurements ($b < 1$)

We now examine the cases corresponding to limited precision, which corresponds to measurability $b < 1$. As b decreases and the measurements become noisier, both the Leggett-Garg inequality violation and the optimality of the metrological scenario are progressively degraded.

In Fig. 4.1(b), we have plotted $F(\theta)$, $C(\theta)$ and $K(\theta)$ for $b = 0.99$. This correspond to a "quasi-projective" measurement. We now observe that the Fisher information is zero at $\theta = n\pi$. This drastic transition observed in this specific model is the consequence of the general relationship between the correlation function and the Fisher information given by Eq. (4.9). As discussed above, this "collapse" of the Fisher information induced by a noisy measurement occurs because $\theta = n\pi$ are common extremum of C and F.

This observation further suggests that the Leggett-Garg inequality violation at the maximum Fisher information is a hallmark of the robustness of the latter against noise.

In this way, we have obtained, in the framework of this model, a connection between the points where invasiveness is witnessed and those corresponding to favorable metrological scenarios. From our results, one can see that the generalization of such a connection between Leggett-Garg inequality and metrological scenarios to other physical models deserves future investigations.

4.3.3 Discussion

Our model sheds light on the relationship between the quantum Fisher information and quantum invasiveness. Some physical insight about this connection was already given in Ref. [Fröwis and Dür, 2012] where, by taking into account a "no-signaling in time condition" [Kofler and Brukner, 2013], the authors argued that quantum states with large $\mathcal{F}_Q$ are necessary for Leggett-Garg inequality violation with large measurement uncertainties.

In order to further investigate this point, we plotted F, K_{LG} and $\mathcal{F}_Q$ as a function of b for fixed values of θ in Fig. 4.2. Specifically, in Fig. 4.2(a), we have fixed $\theta/\pi = 0.95$, a value that allows the violation of the Leggett-Garg inequality for $b > 0.94$. We see that both $\mathcal{F}_Q$ and F increase monotonically as b increases and F approaches its optimal value, $\mathcal{F}_Q$, in the region where Leggett-Garg inequality is violated. On the other hand, in Fig. 4.2(b), we take $\theta/\pi = 0.34$ so that no violation of the Leggett-Garg inequality can occur. Note that $\mathcal{F}_Q$ remains the same as a function of b, as $\mathcal{F}_Q$ does not depend on θ. It is thus clear that large QFI is not a sufficient condition for the Leggett-Garg inequality violation.

Note as well that, in Fig. 4.2(b), the Fisher information increases monotonically as b increases but it does not reach its optimal value, $\mathcal{F}_Q$. In order to investigate further the relationship between the Fisher information and the Leggett-Garg inequality violation, we plot in Fig. 4.3 the normalized Fisher information $F/\mathcal{F}_Q$ versus the absolute value of the Leggett-Garg parameter $|K_{LG}|$. See caption for details.

We see that both the maximum (normalized) Fisher information and the maximum of $|K_{LG}|$ monotonically increase with b. Furthermore, note that $F/\mathcal{F}_Q$ at the point of maximal violation of the Leggett-Garg inequality (solid magenta line) is a monotonically increasing function of the violation itself. We can also see that, even though the maximization of F and $|K_{LG}|$ are generally incompatible, violation of K_{LG} is necessary to access the nearly optimal regime of $F/\mathcal{F}_Q$ above ≈ 0.82. Finally, we see that, when the Leggett-Garg inequality is violated, there is a lower bound for the Fisher information, given by $F/\mathcal{F}_Q \gtrsim 0.27$, thus Leggett-Garg inequality violation guarantees a non-trivial minimum metrological precision. Conversely, when the Leggett-Garg inequality is not violated, the Fisher information can be arbitrarily small and vanish for specific parameter settings.

4.4 Discussion about measures of macroscopic coherence and relationship with invasiveness

Coherence is an intrinsic quantum property, which is directly related to the notion of quantum superposition. As discussed before in this thesis, *coherence* terms are those non-diagonal terms of a density operator, which are related to nonclassical phenomena such as quantum interference. The study of coherence of quantum states and its quantification within the context of *resource theories* [Coecke et al., 2016] has received considerable attention over the last few years [Girolami, 2014, Baumgratz et al., 2014, de Vicente and Streltsov, 2017, Marvian and Spekkens, 2016]. A review of these efforts can be found in Ref. [Streltsov et al., 2016].

Here, we will focus on the notion of *macroscopic coherence*, which, in the same manner as coherence, will also be discussed within the context of a resource theory. Loosely speaking, measures of macroscopic coherence also take into consideration a definition regarding the macroscopicity of the quantum state [Korsbakken et al., 2007, Korsbakken, J. I. et al., 2010, Nimmrichter and Hornberger, 2013, Fröwis et al., 2016, Marquardt et al., 2008, Kwon et al., 2016, Yadin and Vedral, 2016, Leggett, 2016]. This is the reason why they are called "macroscopic".

In the following, we will set the context for the discussion of measures of macroscopic coherences by presenting some concepts on resource theories.

Some concepts on resource theories

We will here briefly highlight some elements and concepts of resource theory which will be used in the remainder of this chapter [Yadin and Vedral, 2016, Baumgratz et al., 2014]:

- *Free states*: states containing no resource.
- *Free operations* $\mathcal{E}$, given a state ρ, are defined as

$$\mathcal{E}(\rho) = \sum_{\alpha} K_{\alpha}^{\dagger} \rho K_{\alpha}, \tag{4.20}$$

  where K_α are Kraus operators satisfying $K_\alpha^\dagger K_\alpha \leq \mathbb{I}$, in such a way that $\mathcal{E}$ is defined as a completely positive trace-non-increasing map. A free operation is defined as *any* quantum operation which is incapable of creating resource.
- Finally, a *measure* or *monotone* of the resource must give zero for free states and never increase under free operations.

As we will see in the following, the measure or *monotone* proposed in Ref. [Yadin and Vedral, 2016] is defined as the quantum Fisher information $\mathcal{F}_Q(\rho, H)$ of a quantum state ρ which undergoes a transformation governed by a Hamiltonian H, such as $\rho(\theta) = e^{-iH\theta}\rho e^{iH\theta}$, where θ is the time evolution.

4.4.1 Yadin and Vedral's measure of macroscopic coherence

In Ref. [Yadin and Vedral, 2016] the notion of coherence is introduced by taking into account the definition of a quantity called δ-*coherence*. This definition is associated with a superposition of the eigenstates $|e_i\rangle$ and $|e_j\rangle$: given an observable H, and the coherent superposition of its eigenstates $|e_i\rangle$ and $|e_j\rangle$, then $\delta_{ij} \equiv |e_i - e_j|$. Roughly speaking, for this measure, the notion of macroscopicity is captured by giving more weight to superpositions involving eigenstates of H to which are associated the largest possible difference between the corresponding eigenvalues. The definition of macroscopicity here is therefore clearly associated with a notion of distance defined by δ, *i.e.* the difference between the eigenvalues of the observable H.

In order to introduce this measure, let us consider a quantum state expanded in the basis of eigenstates of H, $\rho = \sum_{i,j} \rho_{ij} |e_i\rangle \langle e_j|$, in such a manner that the part containing the δ-coherence reads

$$\rho^{(\delta)} = \sum_{i,j:\ e_i - e_j = \delta} \rho_{ij} |e_i\rangle \langle e_j| . \tag{4.21}$$

In this way, the entire quantum state can be expressed as

$$\rho = \sum_{\delta} \rho^{(\delta)}. \tag{4.22}$$

with $\delta \in \Delta = \{e_i - e_j\}_{i,j}$, the set with all the differences between the eigenvalues of H.

Hence, in the context of resource theories and considering coherence as the resource, let us assume that a reasonable measure $\mathcal{M}$ of macroscopic coherence is expected to satisfy the following properties:

(i) $\mathcal{M}(\rho) \geq 0$ *and* $\mathcal{M}(\rho) = 0 \leftrightarrow \rho = \rho^{(0)}$.

(ii) For a deterministic free operation $\mathcal{E}$ *- i.e.,* $\mathrm{Tr}(\mathcal{E}(\rho)) = 1$, $\mathcal{M}(\rho) \geq \mathcal{M}(\mathcal{E}(\rho))$.

(iii) Also, for $\mathcal{E} = \sum_\nu \varepsilon_\nu$, $\mathcal{M}(\rho) \geq \sum_\nu p_\nu \mathcal{M}(\sigma_\nu)$, *where the outcome* $\sigma_\nu = \mathcal{E}_\nu(\rho)/p_\nu$ *occurs with probability* $p_n u = \mathrm{Tr}\mathcal{E}_\nu(\rho)$.

(iv) $\mathcal{M}(\sum_i p_i \rho_i) \leq \sum_i p_i \mathcal{M}(\rho_i)$.

(v) Let $|\psi\rangle = \frac{1}{\sqrt{2}}(|e_i\rangle + |e_j\rangle)$ *and* $|\phi\rangle = \frac{1}{\sqrt{2}}(|e_k\rangle + |e_l\rangle)$. *If* $|e_i - e_j| > |e_k - e_l|$ *then* $\mathcal{M}(|\psi\rangle \langle\psi|) > \mathcal{M}(|\phi\rangle \langle\phi|)$.

The quantum Fisher information is shown to satisfy all the properties (i)-(v). These conditions are not independent, since (iii) and (iv) imply (ii). In Appendix B, we provide a proof that the quantum Fisher information fulfils the conditions described above by following the proof sketched in Ref. [Yadin and Vedral, 2016].

The quantum Fisher information is therefore a measure of *macroscopic* coherence. As mentioned above, in this measure, the notion of macroscopicity is captured by giving higher weight to superpositions of eigenstates associated to larger δ's, as one can see from condition (v).

Now, we will finally discuss the relationship of this measure with our model. Our results suggest an interconnection between invasiveness (which is related to the parameter b, see chapter 3) and the present measure of macroscopic coherence. This is discussed in the previous section and depicted in Fig. 4.2, since this measure corresponds to the quantum Fisher information, $\mathcal{F}_Q(\rho, H)$, with $\rho = \hat{\rho}_+$. Hence, as the measurability b increases, both the absolute value of the Leggett-Garg parameter and the quantum Fisher information increase. In this way, as suggested by our model within the context of the parallel between metrological and the Leggett-Garg scenarios, when the Leggett-Garg inequality is violated, the preparation states associated with this violation also have large macroscopic coherences associated to them. However, as we have also seen in the previous section, the inverse does not hold, *i.e.*, there are preparation states which, in despite of having large macroscopic coherence, do not violate the Leggett-Garg inequality.

4.5 Conclusion

We have established a connection between temporal correlations, involved in Legget-Garg inequality tests, and the Fisher information associated with a specific metrological scenario.

In particular, guided by the general expression of the Fisher information in terms of two-time correlation functions, we established that the precision of the estimation is very fragile against noise unless accompanied by Leggett-Garg inequality violation. In addition, and looking at a specific example, we showed that large quantum Fisher information is not sufficient for violating the Leggett-Garg inequality.

We also illustrated how violation of Leggett-Garg inequality may set a non-trivial lower bound for the precision of parameter estimation while, on the other hand, large Leggett-Garg inequality violations may enable nearly optimal parameter estimation. The ultimate precision limit in which Fisher information and quantum Fisher information coincide may only be achieved under violation of the Leggett-Garg inequality. Generalization of such intriguing connections between measurement invasiveness and sensitivity beyond specific models certainly deserves further investigation.

Finally, we discuss, through our model, a relationship between invasiveness and the quantum Fisher information, and also with a measure of macroscopic coherence.

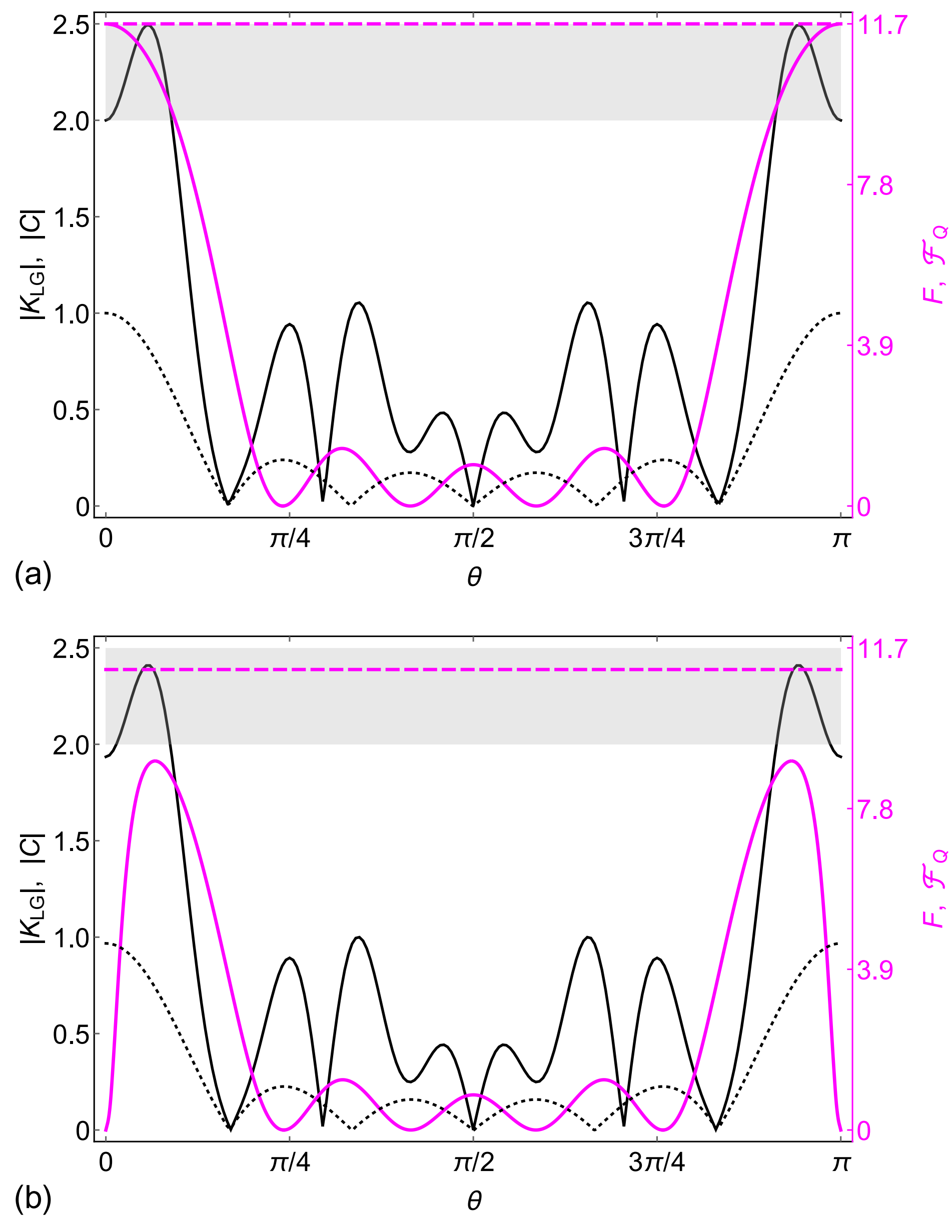

Figure 4.1: Plots of Fisher information F (solid magenta line, scaled to the right vertical axis), quantum Fisher information $\mathcal{F}_Q$ (dashed magenta line, scaled to the right vertical axis), absolute value of the two-time correlation C (dotted black line, scaled to the left vertical axis) and absolute value of K_{LG} (solid black line, scaled to the left vertical axis), as a function of θ, for (a) $b = 1$ and (b) $b = 0.99$. The Leggett-Garg inequality violation region (relative to the left vertical axis) is shaded in light gray. All the plotted quantities are dimensionless.

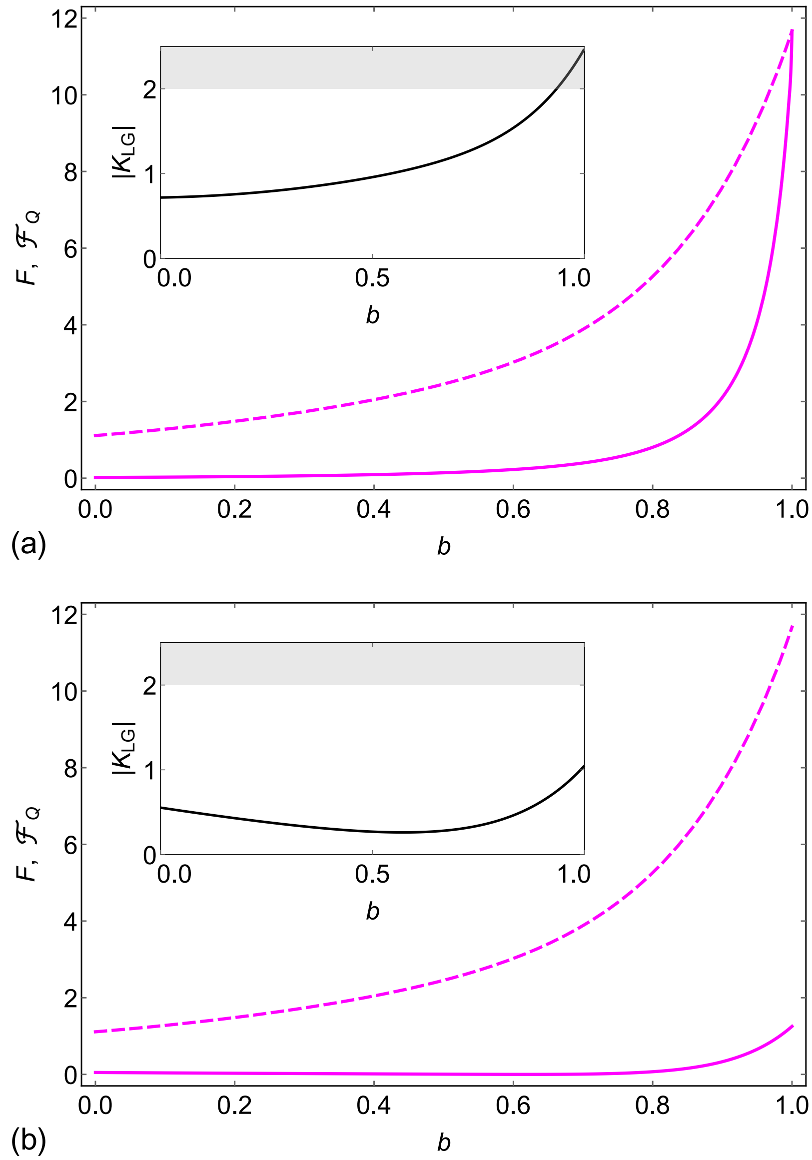

Figure 4.2: Plots of Fisher information F (solid magenta line, scaled to the right vertical axis), quantum Fisher information $\mathcal{F}_Q$ (dashed magenta line, scaled to the right vertical axis), absolute value of the two-time correlation C (dotted black line, scaled to the left vertical axis) and absolute value of K_{LG} (solid black line, scaled to the left vertical axis), as a function of θ, for (a) $b = 1$ and (b) $b = 0.99$. The LGI violation region (relative to the left vertical axis) is shaded in light gray. All the plotted quantities are dimensionless.

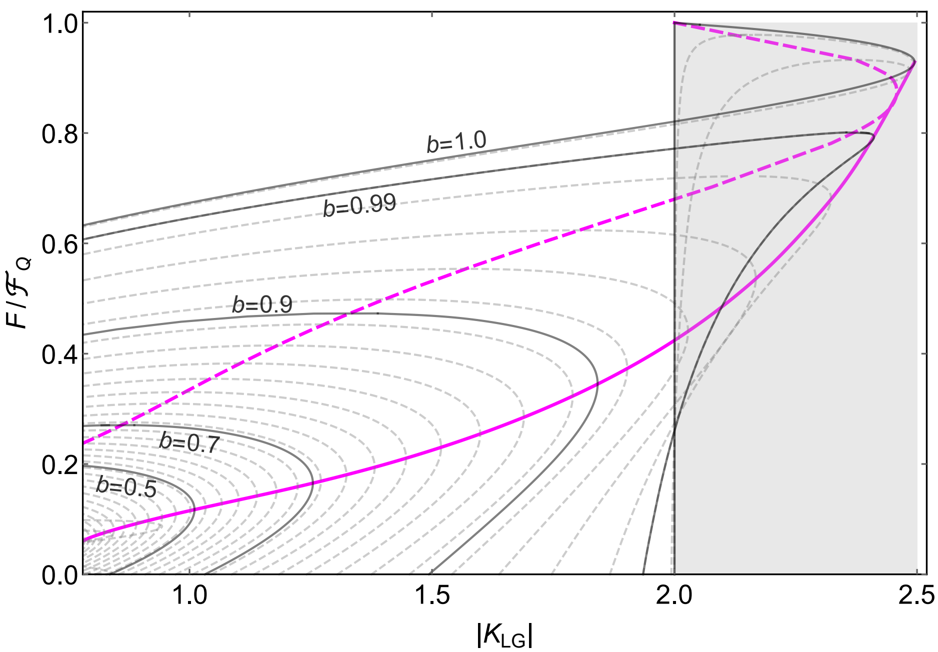

Figure 4.3: Normalized Fisher information, $F/\mathcal{F}_Q$, versus the absolute value of the Leggett-Garg parameter $|K_{LG}|$. The dashed gray lines are contours at fixed b for all $\theta \in [0, \pi/2]$. Specific contours at $b = 0.5, 0.7, 0.9, 0.99, 1.0$ are highlighted as solid dark gray lines. The solid magenta line connects the points at the optimal θ maximizing the Leggett-Garg inequality violation, while the dashed magenta line connects the points at the θ maximizing instead the Fisher information. The Leggett-Garg inequality violation region is shaded in light gray. All the plotted quantities are dimensionless.

Chapter 5

An experimental proposal for testing measurement noninvasiveness

In this chapter, we explore an inequality based on the non-disturbance condition. This is an alternative to the Leggett-Garg inequality which also rules out measurement noninvasiveness, allowing one to argue against the possibility of explaining its violation as a result of classical disturbance, instead of a nonclassical effect. In this way, by using this inequality, we propose an experimental protocol which would allow one to witness measurement invasiveness in systems constituted of N spin-j particles. First, we discuss the simpler case of spin $1/2$ systems, and then generalize for arbitrary spin-j. In both cases, we show that quantum theory predicts violation of the inequality.

5.1 Introduction

So far, we have addressed a fundamental aspect of the frontier between classical and nonclassical effects, related to the notion of measurement invasiveness. Measurements of physical systems, which permit one to obtain information about their properties, presuppose their interaction with a measurement device. However, classical physics assumes *measurement noninvasiveness*, which is to say that, in principle, one can perform measurements on classical systems with arbitrarily small disturbance on their evolution. Conversely, one aspect of the nonclassicality of physical systems is invasiveness, meaning that measurements on these systems often affects their subsequent evolution and which cannot be explained by classical theory.

For example, measurement invasiveness can be illustrated, within the context of the Copenhagen interpretation of quantum theory, by the so-called concept of *collapse*. According to this concept, a quantum superposition of outcomes is reduced to a single one of these results when the system is measured, with probability of obtaining that particular outcome given by the Born rule. The non-deterministic nature of this scenario illustrates the contrast between quantum description and classical physics in regards to measurement processes. More generally, as pointed out earlier in this thesis, fundamental questions and problems related to the measurement process within the scope of the different interpretations of quantum formalism are at the core of the “quantum measurement problem” [Leggett, 2002].

In this chapter, we will present some protocols for testing the Leggett-Garg inequality and discuss how they can help verify that, whenever the Leggett-Garg inequality is violated in an experiment, this is related to measurement invasiveness. Then, by exploring a specific protocol based on the *non-disturbance condition* [Knee et al., 2016], we will develop a proposal for a test of noninvasiveness for spin-j systems.

5.2 Leggett-Garg experimental tests and the clumsiness loophole

An experiment must always be capable of demonstrating convincingly that an experimental violation of the Leggett-Garg inequality is a proof of invasiveness, *i.e.*, that the violation is due to a nonclassical effect. In order to address this issue, one must be able to devise strategies in order to avoid or at least minimize the possibility of the Leggett-Garg inequality violation being explained in terms of classical *clumsiness*, *i.e.* classically invasive measurements or errors present in the experiment.

In fact, as pointed out in Ref. [Wilde and Mizel, 2012], it is, in principle, impossible to definitively prove that a measurement device is not clumsy. Even if a measurement device is not clumsy for a number of tests, one cannot be prove that it would not be for others. Put differently, the hypothesis that a measurement device is not at all clumsy can always be falsified, but cannot be shown to be definitively true. This problem is usually referred as the *clumsiness loophole*.

In the course of the last seven years, there have been a number of experimental tests of measurement noninvasiveness [Xu et al., 2011, Goggin et al., 2011, Athalye et al., 2011, Souza et al., 2011, Knee et al., 2012, Dressel et al., 2011, Emary et al., 2012, Palacios-Laloy et al., 2010, Groen et al., 2013, Robens et al., 2016, Wang et al., 2017a, Wang et al., 2017b]. Ref. [Emary et al., 2014] contains a review of some of these realizations. As we have pointed out above, the conclusions drawn from these tests inevitably suffer as a result of the clumsiness loophole, even though there have recently been outstanding improvements permitting to reduce the effects of this issue [Knee et al., 2016, Wang et al., 2017b, Robens et al., 2016]. In the following, we will review the protocols and strategies most commonly employed, in order to reduce the effects of the clumsiness loophole, up until the current time. The last of these, called the *non-disturbance condition*, will receive particular attention in the experimental proposal developed in the present chapter.

5.2.1 A protocol addressing the clumsiness loophole

In Ref. [Wilde and Mizel, 2012], a strategy is devised in order to minimize the effects of classical clumsiness in tests of the Leggett-Garg inequality. This strategy is based on the definition of *adroit measurement*. As an introduction to this definition, consider, for instance, the experiment represented in the first line of Fig. 5.1, where a dichotomic observable Q is measured at times t_i, $i = 1, 2, 3$. We will denote the outcome of a measurement of the observable Q at time t_i by $Q_i = Q(t_i)$. The second measurement at t_2 is said to be adroit if "it does not have any effect on the joint probability distribution of the outcomes of the first and third measurements" [Wilde and Mizel, 2012].

In order to formalize this notion, consider that the outcomes of the first and third measurement are $Q_1 = a$ and $Q_3 = c$. In this case, the second measurement is ϵ-adroit if the following inequality is satisfied:

$$\sum_{a,c} |p(a,c|\text{2nd measurement is performed}) \\ - p(a,c|\text{2nd measurement not performed})| \leq \epsilon, \tag{5.1}$$

where $p(a,c)$ are joint probabilities of obtaining the outcomes a and c.

Now, given that the 2nd measurement is confirmed to be ϵ-adroit, it is not unreasonable to assume that two ϵ-adroit measurements yield a 2ϵ-adroit composite measurement - this is called *closure of adroit measurements*. However, if there is an abrupt effect provoked by the 2nd measurement which is not revealed by the ϵ-adroitness test, it is in principle possible for two apparently ϵ-adroit measurements to *collude* and cause a strong disturbance. In this case, inequality (5.1) would be violated due to "undetected" clumsiness in the ϵ-adroit test. This protocol does not rule out this possibility, which, in the authors' words, is "unnatural".

It is also described in Ref. [Wilde and Mizel, 2012] how adroit measurements can be employed in a Leggett-Garg inequality test, helping one to argue against the possibility of classical disturbances whenever one obtains a violation. Suppose the experiment depicted in the first line of Fig. 5.1(counting from the top) is carried out (counting from the top) with the input state ρ and considering $Q_2 = A$, and its ϵ-adroitness is determined with $Q_1 = M'$, and $Q_3 = M''$. Then, one also establishes the ϵ-adroitness of measurements of $Q_2 = B$ and $Q_2 = C$, in the conditions illustrated in the second, third and fourth lines of Fig. 5.1.

Finally, one performs a Leggett-Garg test described in chapter 2, such that

$$\langle Q_1 Q_2 \rangle + \langle Q_2 Q_3 \rangle - \langle Q_1 Q_3 \rangle \leq 1, \tag{5.2}$$

also considering $Q_1 = M'$, and $Q_3 = M''$ and the input ρ, as illustrated in the last line of Fig. 5.1. This test is such that, in the realizations to measure the correlation $\langle Q_1 Q_3 \rangle$, one carries out neither the "box" of measurements ABC, nor the measurement of Q_2. Conversely, both the "box" of measurements ABC and Q_2 are measured in the realizations to determine $\langle Q_1 Q_2 \rangle$ and $\langle Q_2 Q_3 \rangle$. Finally, by invoking the closure of adroit measurement (since all the measurements involved in the realizations have been previ-

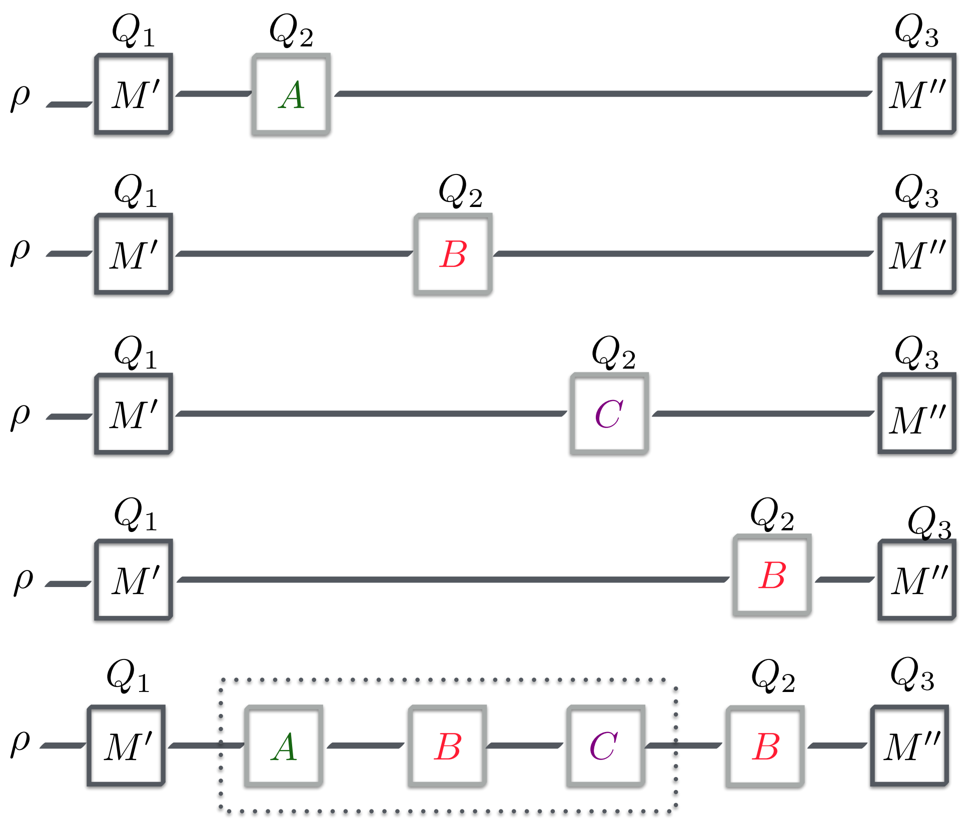

Figure 5.1: Illustration of the protocol devised in order to *tight* the clumsiness loophole, adapted from Ref. [Wilde and Mizel, 2012]. First to fourth line (counting from the top): sketch of the experiments in which the ϵ-adroitness of the measurements of the observables are individually established, considering the input state ρ and $Q_1 = M'$ and $Q_3 = M''$. Finally, in the last line, we have a representation of the measurements used in a Leggett-Garg test. The "box" of measurements is performed whenever Q_2 is also performed. By assuming the closure of adroit measurements, one can reasonably claim that, if the a violation is observed, it is due to a nonclassical effect.

ously determined to be ϵ-adroit), whenever one observes a Leggett-Garg inequality violation, one can therefore reasonably attribute this violation to invasiveness.

An example of violation using this protocol can be found in Ref. [Wilde and Mizel, 2012] for a qubit system.

5.2.2 Ideal non-negative measurements

The proposition of protocols relying on *ideal non-negative measurements* [Leggett and Garg, 1985, Leggett, 2008, Leggett, 1988], is another strategy which has been employed in many experiments with the goal of providing elements which would allow one to argue against the possibility of explaining the Leggett-Garg violation as having classical disturbance as its cause [Leggett and Garg, 1985]. Indeed, this condition was proposed in 1985 by Leggett and Garg in their proposition of the inequality with a system called *flux qubit*. The detailed description of this system and proposition can be found in Ref. [Leggett and Garg, 1985].

The concept of non-negative measurements can be illustrated by using a qubit system $\{|0\rangle, |1\rangle\}$. Suppose that, in a experiment, we use a measurement device which cannot interact with the state $|0\rangle$, whilst it can only interact (and then "click" with a hundred percent probability) with the system's state $|1\rangle$. Then, whenever the device *does not* click, one can deduce that the system was in the state $|0\rangle$ immediately before the measurement. Now, by using a device which cannot interact with the state $|1\rangle$, but that does detect the system in state $|0\rangle$, one can obtain the complete set of data in a non-invasive way.

In summary, the basic principle of an ideal non-negative measurement is to reject the set of data obtained whenever the measurement device interacts with the system, *i.e.*, whenever the detector clicks, for instance. Therefore, one can be sure that all the data collected in the experiment is obtained in situations where there is no interaction of the measurement device with the system, thus avoiding classical clumsiness.

5.3 The non-disturbance condition

We will now review the protocol proposed in Ref. [Knee et al., 2016], based on a condition called *quantum witness* [Schild and Emary, 2015]. We also describe how, ideally, it avoids the clumsiness loophole. This involves the test of what was defined by the authors as the *non-disturbance condition*. The definition of the non-disturbance condition is given in the context of the illustration of Fig. 5.2, where the measurement of the observable Q, which has g and e as possible outcomes, is performed at t_2.

At $t = 0$, the system is in a preparation associated with the outcome g, the eigenstate $|g\rangle$. Then, one prepares the state ρ by applying a unitary transformation U_1 to the initial state. In the upper part of Fig. 5.2, a

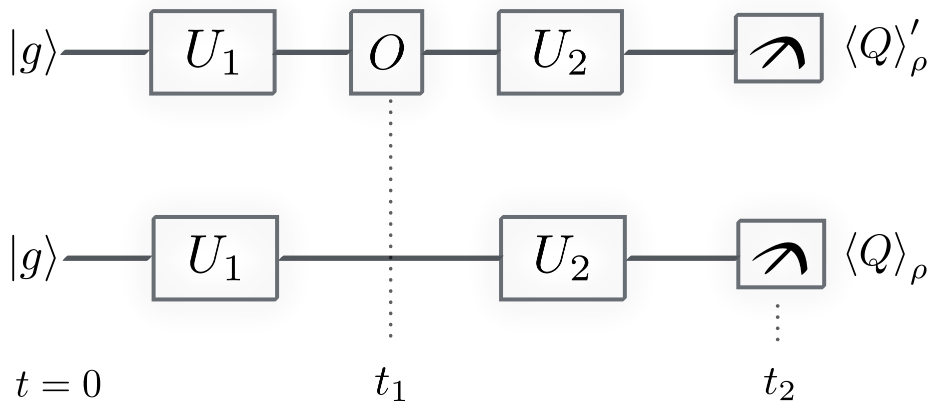

Figure 5.2: Scheme of the main experiment: in the upper part, a system initially in the state $|g\rangle$ at $t=0$ is subjected to the transformation U_1, and then to the measurement operation O at t_1. Finally, the measurement of the observable Q is performed at t_2. The same realization is considered in the lower part of the figure, except for the fact that O is not carried out at t_1.

measurement operation O is performed at t_1. Such measurement can be a *blind measurement* [Schild and Emary, 2015]. A measurement is called blind whenever one does not record or have access to the measurement results.

Next, the system is subjected to the transformation U_2, with Q being finally measured at t_2. By repeating many times both experiments, sketched in the upper and lower part of Fig. 5.2, one is able to collect statistics and finally obtain the expectation values $\langle Q\rangle'_\rho$ and $\langle Q\rangle_\rho$, respectively. In the upper part, the prime indicates that the measurement operation O at t_1 is performed. In the lower part of Fig. 5.2, the same experimental realization is considered, except for the fact that O is not performed. The definition of the non-disturbance condition is then given by

$$d_\rho \equiv \langle Q\rangle_\rho - \langle Q\rangle'_\rho = 0. \tag{5.3}$$

Consequently, the non-disturbance condition is verified only if the measurement operation O has no significant effect on the statistics of the last measurement.

In a recent paper [Wang et al., 2017b], K. Wang and co-authors generalize this protocol by replacing O by a general Kraus map. Therefore, even a unitary operation would be suitable for replacing the measurement operation O. The interpretation of this generalization is based on the fact that, in quantum theory, a global quantum phase of a state have a null effect on quantum systems, since it cannot be detected. However, if no quantum superposition of eigenstates preparations is possible (according to quantum theory, the states involved in a quantum superposition pick up relative phases) and one has just a statistical or incoherent mixture, then $d_\rho = 0$ must be obtained. Hence, the violation of (5.3) would allow one to verify nonclassical behaviour associated with the invasiveness of O.

Proof of the non-disturbance condition

The proof of the non-disturbance condition follows immediately from the derivation of the quantum witness in Ref. [Schild and Emary, 2015]. In order to derive the non-disturbance condition in this general case, consider two observables A and B, measured at times $t = 0$ and $t = T > 0$, respectively. In the general case, where the measurement of observable A is a blind measurement, we represent its possible outcomes by a_i. Suppose one measures the observable B, obtaining always the outcome b. The quantum witness is then defined as follows

$$W = P(b) - P'(b), \tag{5.4}$$

where $P'(b) = \sum_i P(b|a_i)P(a_i)$, with $P(b|a_i)$ the conditional probability of obtaining the outcome b, given that the outcome a_i was previously obtained. W is then expected to be zero if the measurement of observable A does not affect the probability of obtaining the outcome b at a later time.

5.3.1 Control-experiment: ruling out classical clumsiness

A control-experiment, the scheme of which is depicted in Fig. 5.3, is set in parallel to the main experiment, with the goal of avoiding classical disturbances of the measurement at t_1.

In Ref. [Knee et al., 2016] a scheme similar to Fig. 5.2 is considered, with the difference that the transformation U_1 is not applied. One can then write the *classical* non-disturbance conditions

$$\begin{aligned} d_g &= \langle Q \rangle_g - \langle Q \rangle'_g \\ d_e &= \langle Q \rangle_e - \langle Q \rangle'_e , \end{aligned} \tag{5.5}$$

where the index g or e indicates the corresponding preparations. Therefore, if d_g or d_e is not equal to zero, it follows then that O induces a classical disturbance.

Thus, taking into account the control-experiments and by assuming that they can reasonably rule out the classical disturbances, nonclassical effects can be witnessed only if the following inequality is violated:

$$\min(d_g, d_e) \leq d_\rho \leq \max(d_g, d_e). \tag{5.6}$$

In this way, by associating the preparations with the eigenstates of a given observable, effects of classical disturbances in the experiment can be ruled out. This follows from the fact that eigenstates of the observable considered, having definite outcomes associated with them, can be related with *classical states*. Therefore, by performing these experiments, one can determine the classical clumsiness resulting from the test of the aforementioned classical preparations.

5.4 Testing measurement noninvasiveness within spin-j systems

Here, we will employ the protocol described above in order to propose an experimental test of measurement noninvasiveness in systems constituted of N spin-j particles. First, we will consider spin 1/2 systems, and then

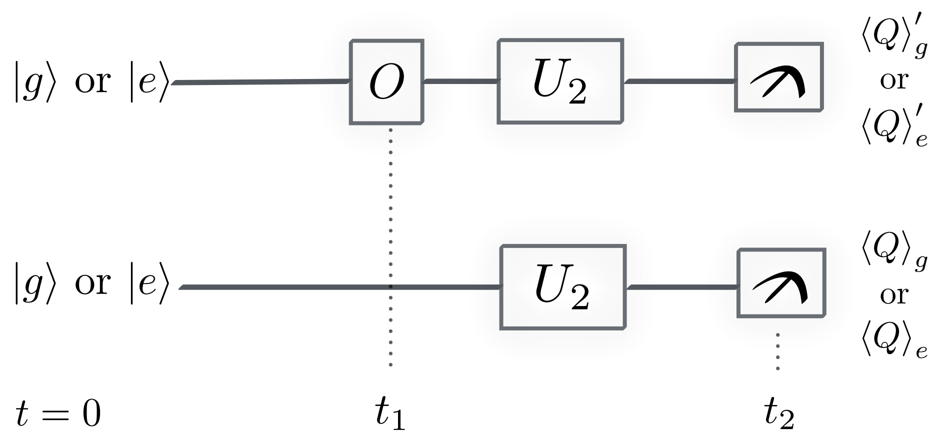

Figure 5.3: Scheme of the control experiment: in the upper part, a system initially in the state $|g\rangle$ at $t = 0$ is subjected to the measurement operation O at t_1. The measurement of the observable Q is performed at t_2. The same realization is considered in the lower part of the figure, except for the fact that O is not carried out at t_1

generalize for arbitrary spin-j. By judiciously choosing the measurement operation O and the transformations U_1 and U_2, we will show that quantum theory predicts a maximal violation equal to the number of particles N, for arbitrary spin-j systems. Such large violations would possibly be more effective in order to overcome issues as classical clumsiness in the experiment.

5.4.1 N Spin $1/2$ particles

We will first consider a two-level system constituted of N spin $1/2$ particles, and define the observable Q as

$$Q = \sum_{k}^{N} |e\rangle_k \langle e| - |g\rangle_k \langle g| . \tag{5.7}$$

Hence, the measurement of Q determines the populations of the eigenstates $|e\rangle_k$ and $|g\rangle_k$, where $|e\rangle$ is associated with the spin eigenstate of the k-th particle $|e\rangle_k \to |1/2\rangle$ and $|g\rangle_k \to |-1/2\rangle$. As mentioned above, the measurement of $\hat{Q}$ can be accomplished by performing a Stern-Gerlach like experiment such as described in chapter 3, for instance. In what follows, the other elements of the main and control experiments illustrated in Figs. 5.2 and 5.3 are defined. We consider the transformations $U_1 = U_2 = U$ as rotations of $\pi/2$ around the $\hat{y}$-axis, *i. e.*,

$$U = (e^{-i\frac{\pi}{2}\sigma_y})^{\otimes N}, \tag{5.8}$$

where σ_y is the Pauli matrix [Cohen-Tannoudji et al., 1973] associated with the y-component of the spin 1/2. As a result, when U is applied to each one of the one-particle eigenstates $|g\rangle$ and $|e\rangle$, one obtains

$$\begin{aligned} |g\rangle &\to \frac{1}{\sqrt{2}}(|g\rangle + |e\rangle) \\ |e\rangle &\to \frac{1}{\sqrt{2}}(|e\rangle - |g\rangle). \end{aligned} \tag{5.9}$$

Local superpositions are therefore generated. For instance, by considering the system's state as

$$|g\rangle \otimes |g\rangle \otimes |g\rangle \otimes \cdots \otimes |g\rangle \equiv |g\rangle^{\otimes N}, \tag{5.10}$$

and applying the rotation U on it, one obtains

$$\begin{gathered} |\psi\rangle = \left(\frac{1}{\sqrt{2}}|g\rangle + |e\rangle\right) \otimes \left(\frac{1}{\sqrt{2}}|g\rangle + |e\rangle\right) \otimes \cdots \otimes \left(\frac{1}{\sqrt{2}}|g\rangle + |e\rangle\right) = \\ \left(\frac{1}{\sqrt{2}}|g\rangle + |e\rangle\right)^{\otimes N}. \end{gathered} \tag{5.11}$$

The measurement operation O is defined as a projector onto the system's ground state $|g\rangle^{\otimes N}$:

$$O = (|g\rangle\langle g|)^{\otimes N} \tag{5.12}$$

The accomplishment of such a measurement operation can be achieved, for example, through *spin relaxation* [Pasquiou et al., 2011]. In this way, the outcome of this measurement is always the system's collective ground state 5.10.

Now, since all the elements of Figs. 5.2 and 5.3 were defined and identified, we are therefore able to discuss individually the experiments to which they refer. We start by the control experiment of Fig. 5.3. In this case, one can easily see that $\langle Q\rangle_g' = 0$ and $\langle Q\rangle_g = 0$. Similarly, $\langle Q\rangle_e' = 0$ and $\langle Q\rangle_e = 0$. This is a consequence of the fact that all the system's output states, both in the lower an upper part of the control experiment of Fig. 5.3 are the superpositions

$$\left(\frac{1}{\sqrt{2}}\left|g\right\rangle \pm \left|e\right\rangle\right)^{\otimes N}. \tag{5.13}$$

As a result, one obtains

$$d_g = d_e = 0. \tag{5.14}$$

Accordingly, it suffices that $d \neq 0$ in order to violate inequality (4.2). Note that the collective preparation states considered in the control experiments of Fig. 5.3 are $\left|g\right\rangle^{\otimes N}$ and $\left|e\right\rangle^{\otimes N}$. Since $U_1 = U_2 = U$ are local transformations, it is easy to see that all product states of the form

$$\left|g(e)\right\rangle^{\otimes N},$$

where $\left|g(e)\right\rangle$ can be either the $\left|g\right\rangle$ or $\left|e\right\rangle$, give $d_{g(e)} = 0$ as well.

We now turn our attention to the main experiment of Fig. 5.2. Considering the experimental realization in the upper part of the illustration of the experiment, the state measured at t_2 is

$$\left(\frac{1}{\sqrt{2}}\left|g\right\rangle + \left|e\right\rangle\right)^{\otimes N}. \tag{5.15}$$

Therefore, $\langle Q\rangle_\rho' = 0$. On the other hand, for the lower part, the state measured at t_2 is

$$\left|e\right\rangle^{\otimes N}. \tag{5.16}$$

In this way, $\langle Q\rangle_\rho = N$, so that the non-disturbance condition for the main experiment will be given by

$$d_\rho = N. \tag{5.17}$$

Hence, inequality (4.2) is potentially violated in this case, and one can see that the obtained violation scales linearly with the total number of particles N.

To conclude this discussion, we show that if statistical mixtures ρ are prepared,

$$\rho = \left(\frac{1}{2}(|g\rangle\langle g| + |e\rangle\langle e|)\right)^{\otimes N}, \tag{5.18}$$

they cannot violate inequality (4.2), supposing that the elements ($U_2 = U$ and O) are kept the same as before (note that we do not use U_1 here, but instead prepare a statististical mixture). This is due to the fact that, in the lower part of the sketch of the main experiment, we would have

$$U_2^{\dagger}\rho U_2 = \rho, \tag{5.19}$$

since a unitary transformation does not change the completely mixed state. Hence, $\langle Q\rangle_\rho = 0$. Now, considering the realization sketched in the upper part of Fig. 5.2, we see that the state measured at t_1 will be $|g\rangle^{\otimes N}$. In consequence, after the application of U_2, the state at t_2 will be the superposition (5.15). Therefore, $\langle Q\rangle'_\rho = 0$. As a result, one obtains $d_\rho = 0$, which shows that violation of the inequality (5.6) is impossible for statistical mixtures.

Finally, one may argue that $d_g = d_e = 0$ are not suitable for experiments [Wang et al., 2017b]. Indeed, there may be errors due to underlying uncontrollable variables in the experiment. The only way of ruling out these errors is via the realization of the control experiments, possibly giving d_g and d_e different from zero. This would then change the conditions for violation.

5.4.2 General case: N spin-j particles

We will now generalize the protocol described above for a system of N spin-j particles, $j \in \mathbb{N}$. This protocol may be possibly implemented in the experiment with cold atoms of chromium ($j = 3$) of the Cold Atoms Group at the Université Paris 13 [Naylor et al., 2016, Naylor et al., 2015, Pasquiou et al., 2011]. We will denote the eigenstates of the $\hat{\alpha}$-component of a single spin, J_α, by $|\alpha, m\rangle$, $m = -j, \ldots, j$.

We will choose the observable Q as

$$Q = \sum_{k}^{N}\left(\sum_{m<0}|z,m\rangle_k\langle z,m| - \sum_{m>0}|z,m\rangle_k\langle z,m|\right). \tag{5.20}$$

Hence, as one can see, $\langle m\,|\,Q\,|\,m\rangle > 0$ for $m < 0$ and $\langle m\,|\,Q\,|\,m\rangle < 0$ for $m > 0$. For $m = 0$, $\langle m\,|\,Q\,|\,m\rangle = 0$.

As above, we consider $U_1 = U_2 = U$ both in the control and main experiments, with U as a local rotation around the $\hat{y}$-axis,

$$U = (e^{-i\frac{\pi}{2}J_y})^{\otimes N}. \tag{5.21}$$

In this way, by applying U to a single-particle eigenstate $|z, m\rangle$, we have

$$|z, m\rangle \to |x, m\rangle \,, \tag{5.22}$$

and if it is applied again to the output $|x, m\rangle$, one obtains

$$|x, m\rangle \to - |z, m\rangle \,. \tag{5.23}$$

Also, similarly to the spin 1/2 case, the measurement operation O is defined as a projector onto the system's ground state, $|z, -j\rangle^{\otimes N}$:

$$O = (|z, -j\rangle \langle z, -j|)^{\otimes N}. \tag{5.24}$$

As discussed before, this measurement operation can be associated with spin relaxation [Pasquiou et al., 2011].

We analyze now the control experiments of Fig. 5.3, which will be realized for each one of the eigenstates $|z, m\rangle$ as inputs at $t = 0$. Therefore, a total of $2j+1$ control experiments must be carried out in order to obtain the associated non-disturbance conditions $d_m = \langle Q\rangle_m - \langle Q\rangle'_m$. One can see that, at t_2, both the lower and upper part of the control experiment of Fig. 5.3, performed with an input state $|z, m\rangle^{\otimes N}$ at $t = 0$, are eigenstates of the x-component of the spin, J_x. These eigenstates $|x, m\rangle$ are superpositions of the eigenstates $|z, m\rangle$, which can be expressed as follows

$$|x, m\rangle = \sum_{m=-j}^{j} c_m \,|z, m\rangle \,, \tag{5.25}$$

with coefficients $c_m \in \mathbb{C}$ satisfying $|c_m| = |c_{-m}|$ (see Appendix A). It follows then that

$$d_m = \langle Q\rangle_m - \langle Q\rangle'_m = 0, \tag{5.26}$$

$\forall$ the m's.

Finally, we consider the main experiment of Fig. 5.2. We suppose that it is carried out with the state $|z, -j\rangle^{\otimes N}$ as input at $t = 0$. In so doing, one obtains $\langle Q\rangle_\rho = -N$, since, as showed in the lower part of Fig. 5.2 and according to (5.22) and (5.23), the application of the transformation

U twice will lead the system's state into the following eigenstate

$$-\,|z,-j\rangle^{\otimes N}.$$

Due to the realization of the measurement operation O at t_1, illustrated in the upper part of Fig. 5.2, it can be easily seen that, similarly to the control experiment, $\langle Q\rangle'_\rho = 0$. As a result, we obtain

$$d_\rho = \langle Q\rangle_\rho - \langle Q\rangle'_\rho = -N. \tag{5.27}$$

Therefore, violation of the inequality 5.6 can be achieved for an arbitrary spin-j system, considering the specific protocol proposed above.

5.5 Discussion about macroscopicity

The superpositions created within the experiment described above are local, as in (5.11), for instance. In this way, entanglement is not taken into consideration here. Therefore, although the system under consideration can be composed of many N particles, one cannot speak of superposition of *macroscopic distinct states* [Leggett, 2002], as it is the case for superpositions of the states as the so-called Greenberger-Horne-Zeilinger (GHZ) state, *i. e.*

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|g\rangle^{\otimes N} + |e\rangle^{\otimes N}). \tag{5.28}$$

This state is also known as an"ideal" N-particle *cat state*.

When the inequality (5.6) is violated, nonclassicality of the N-particle system can be witnessed, which is in this case due to local superpositions. Considering the protocol studied in this chapter, we have seen that $d_\rho = N$ for spin-j systems. After the realization of the control experiments, one may then obtain a large value for the violation of inequality (5.6) in the laboratory, scaling with the number of particles of the system, depending on the result of the control experiments. Note that we assumed that all the N particles are involved in these local superpositions. If it is not the case, then $d_\rho < N$. Therefore, one progressively loses violation of (5.6) by reducing the number of particles involved in the local superpositions.

In Ref. [Leggett, 1980], Leggett introduced a measure of *macroscopic distinctness* of two quantum states. It consists of two quantitative measures named *extensive difference* and *disconnectivity*. The first definition, the extensive difference, consists of the disparity between the values of a relevant extensive quantity for the system in each one of these two states, normalized to some characteristic value of that quantity in a relevant microscopic scale. A related definition for the extensive difference λ for state (5.11) can be given by the definition of the operator Λ:

$$\Lambda = \frac{\sum_i^N |e\rangle_i \langle e| E_e - \sum_i^N |g\rangle_i \langle g| E_g}{E_e - E_g}, \tag{5.29}$$

where $E_{e(g)}$ is the energy of an atom in the state $|e(g)\rangle$. Then, λ can be defined then as

$$\lambda = \langle \Lambda \rangle. \tag{5.30}$$

By setting $E_g = 0$ and $E_e = 1$, (5.29) can be expressed as

$$\Lambda' = \sum_i^N |e\rangle_i \langle e|. \tag{5.31}$$

and therefore,

$$\lambda' = \langle \Lambda' \rangle = n_e \sim N. \tag{5.32}$$

The second definition, disconnectivity, will not be discussed here, since it is related to the notion of *degree of entanglement* [Vedral et al., 1997] and the concept of macroscopic distinct states mentioned in chapter 4, and therefore, is not pertinent here.

To conclude, we see that the violation of inequality (5.6) may be of the order of the extensive difference of the superposition (5.11), *i.e.* of the order of the total number of particles N. In other words, the violation obtained can be of the order of a quantity characterizing a specific aspect of the macroscopicity of quantum systems. As we have seen above, however, the magnitude of the violation will ultimately depend on the realization of the control experiments.

5.6 Conclusion

In this chapter, we introduced a protocol for testing noninvasiveness through the non-disturbance condition in systems constituted of N spin-j particles. We have seen that, within this protocol, in order to address the possibility of classical clumsiness of measurements explanining the violation of the non-disturbance condition instead of a genuine nonclassical effect (invasiveness), control experiments are proposed.

In this way, depending on the control experiments, one can obtain large violations for inequality (5.6), scaling with the system's number of particles N. Therefore, this violation can be of the order of the extensive difference, a quantity characterizing a specific aspect of the macroscopicity of quantum systems.

Chapter 6

Conclusion

Throughout this thesis, we have focused on the study of a specific aspect of the frontier between classical and nonclassical phenomena. Namely, we investigated the nonclassical concept of measurement invasiveness, *i.e.*, the effect that the measurement of a quantum system has on its subsequent evolution, and which cannot be described by classical physics. To do so, we explored the Leggett-Garg inequality and an inequality based on a condition called the *non-disturbance condition*, both involving realizations considering sequential measurements performed on a system as it evolves. We also investigated the relationship of measurement invasiveness with specific definitions of macroscopicity and macroscopic coherence.

In the first part of this work, we proposed a model where the violation of the Leggett-Garg inequality, and therefore measurement invasiveness, can be directly controlled and understood through physically sound parameters. These parameters can be associated with the imprecision of a measurement, which in turn, can be attributed to different physical origins. Furthermore, by using spin-j systems, we showed that violations of the inequality do not depend on the size of the spin (defined as the magnitude of j), and can be modelled solely as a function of a parameter, called *measurability*, which determines the invasiveness or disturbance of a measurement. This model can be used to help understanding and interpreting Leggett-Garg inequality tests, and can be tested experimentally in a number of physical systems, such as Stern-Gerlach-like experiments with inhomogeneous fields, or the orbital angular momentum of photons.

We then investigated an application of measurement invasiveness in the context of quantum metrology. We derived a general expression for the Fisher information as a function of temporal correlations and, guided by this expression, we demonstrated that the precision of parameter estimation is very fragile against noise unless accompanied by the violation of the Leggett-Garg inequality. Furthermore, by using a specific model, we showed that large quantum Fisher information is not sufficient for the violation the Leggett-Garg inequality. By considering spin systems, we illustrated how violation of the Leggett-Garg inequality may set a non-trivial lower bound for the precision of parameter estimation. Conversely, large violations of the Leggett-Garg inequality may enable nearly optimal parameter estimation. The relationship between measures of macroscopic coherence and measurement invasiveness was also explored, suggesting that the violation of the Leggett-Garg inequality is a witness of macroscopic coherence.

Generalization of such intriguing connections between measurement invasiveness and sensitivity beyond specific models certainly deserves further investigation. Also, the results obtained concerning specific definitions of macroscopicity and their relationship with measurement invasiveness may help in the search for a more general and sound definition of macroscopicity in regards to the quantum-to-classical transition.

Finally, we proposed a protocol for testing measurement noninvasiness based on the non-disturbance condition for spin-j systems of arbitrary size. This inequality allows one to argue against the possibility of acrediting its violation to the classical disturbance of measurements. We showed that the maximal violation corresponds to the number of particles which constitutes the system. However, the exact value for the violation will ultimately depend on the presence of classical disturbance in the experiment in which the experiment is performed, which can be detected by performing control experiments. This protocol could possibly be implemented in the experiment with cold atoms of chromium ($j = 3$) of the Cold Atoms Group at the Université Paris 13.

Appendix A

Symmetry of rotations

In order to show that, in chapter 5, the coefficients c_m in (5.25) satisfy $|c_m| = |c_{-m}|$, we will briefly introduce the definition of *Wigner rotation matrices* and demonstrate the symmetry of their elements. The elements of Wigner rotation matrix are the elements of the rotation operator [Morrison and Parker, 1987, Pagaran et al., 2006],

$$\begin{aligned}\mathcal{D}^j_{\mu m} &= \langle j\mu \,|\, \exp(-i\alpha J_z)\exp(-i\beta J_y)\exp(-i\gamma J_x) \,|\, jm\rangle \\ &= \exp(-i\mu\alpha)\,\langle j\mu \,|\, \exp(-iJ_y\beta) \,|\, jm\rangle \exp(-im\gamma) \\ &= \exp(-i\mu\alpha) d^j_{\mu m}(\beta)\exp(-im\gamma),\end{aligned} \tag{A.1}$$

where

$$\begin{aligned}d^j_{\mu m}(\beta) = \left[\frac{(j-m)!(j+\mu)!}{(j+m)!(j-\mu)!}\right]^{\frac{1}{2}} (\cos\frac{\beta}{2})^{(m+\mu)}(\sin\frac{\beta}{2})^{(m-\mu)} \\ \times P^{(m-\mu,m+\mu)}_{j-m}(\cos\beta).\end{aligned} \tag{A.2}$$

The elements $d^j_{\mu m}(\beta)$ define, therefore, the reduced matrix $\hat{\mathbf{d}}(\beta)$.

In (A.2), $P_n^{(n_1,n_2)}(\cos\beta)$ are the Jacobi polynomials given by

$$P_n^{(n_1,n_2)}(\cos\beta) = (n+n_1)!(n+n_2)!$$
$$\times \sum_s \frac{1}{s!(n+n_1-s)(n_2+s)!(n-s)!}(-\sin^2\frac{\beta}{2})^{(n-s)}(\cos^2\frac{\beta}{2})^s, \tag{A.3}$$

where $n_1, n_2, n \in \mathbb{Z}$. The sum over s is taken over all the integers for which the arguments of the factorials are positive.

Finally, it can be shown that $d^j_{\mu m}(\beta)$ obeys the following symmetry [Pagaran et al., 2006]:

$$d^j_{\mu m}(\beta)(\pi-\beta) = (-1)^{j-m} d^j_{-\mu m}(\beta).$$

Therefore, for $\beta = \pi/2$, as it is the case in (5.21), we have

$$d^j_{\mu m}(\pi/2) = (-1)^{j-m} d^j_{-\mu m}(\pi/2).$$

As a result,

$$|d^j_{\mu m}(\pi/2)|^2 = |d^j_{-\mu m}(\pi/2)|^2. \tag{A.4}$$

Therefore, since the coefficients c_m of the superposition (5.25), which results from the application of the rotation (5.21), can be written as

$$|c_m|^2 = |\langle m|\,\hat{\mathbf{d}}\,|m\rangle|^2 = |d^j_{mm}(\pi/2)|^2, \tag{A.5}$$

we have that $|c_m| = |c_{-m}|$.

Appendix B

Quantum Fisher information as a measure of macroscopic coherence

We follow the proof sketched in Ref. [Yadin and Vedral, 2016] that the quantum Fisher information is a measure of macroscopic coherence according to the definition presented in chapter 4. We will reproduce here the proof that the conditions (ii) and (v) are fulfilled. Before this, we will first evaluate some commutators which will be used later. In a similar way as in (4.21), we will first write the Kraus operators in the following form

$$K_\alpha = \sum_{\delta_\alpha} \sum_{(i,j)\sim\delta_\alpha} c_{\alpha,i,j} \left|e_i\right\rangle \left\langle e_j\right|, \tag{B.1}$$

for some $\delta_\alpha \in \Delta$, where $(i,j) \sim \delta_\alpha$ means that $e_i - e_j = \delta_\alpha$.

Then, let us evaluate the following commutator $[H, K_\alpha]$:

$$\sum_{(i,j)\sim\delta_\alpha} c_{\alpha,i,j}[H, \left|e_i\right\rangle \left\langle e_j\right|] = \sum_{(i,j)\sim\delta_\alpha} c_{\alpha,i,j}(e_i - e_j) \left|e_i\right\rangle \left\langle e_j\right| = \delta_\alpha K_\alpha. \tag{B.2}$$

By using the commutation relation above, one can write

$$[H^2, K_\alpha] = 2\delta_\alpha K_\alpha H + \delta_\alpha^2 K_\alpha. \tag{B.3}$$

Now, following Ref. [Gour and Spekkens, 2008], suppose that a system is in a pure state $|\psi\rangle$ and that, in a measurement, the outcome α is obtained.

The system's state will then read

$$|\phi_\alpha\rangle = \frac{K_\alpha}{\sqrt{w_\alpha}} |\psi\rangle , \tag{B.4}$$

where $w_\alpha = \langle \psi \,|\, K_\alpha^\dagger K_\alpha \,|\, \psi \rangle$.

Let us define $V(|\psi\rangle)$ as the variance of the observable H in the state $|\psi\rangle$:

$$\sum_\alpha w_\alpha V(|\psi_\alpha\rangle) = 4 \sum_\alpha \left(\langle \psi \,|\, K_\alpha^\dagger H^2 K_\alpha \,|\, \psi \rangle - \frac{\langle \psi \,|\, K_\alpha^\dagger H K_\alpha \,|\, \psi \rangle^2}{w_\alpha} \right). \tag{B.5}$$

By employing the commutation relations above, we have

$$\sum_\alpha \langle \psi \,|\, K_\alpha^\dagger H^2 K_\alpha \,|\, \psi \rangle = \\ \langle \psi \,|\, H^2 \,|\, \psi \rangle + 2 \sum_\alpha \delta_\alpha \langle \psi \,|\, K_\alpha^\dagger K_\alpha H \,|\, \psi \rangle + \sum_\alpha w_\alpha \delta_\alpha^2, \tag{B.6}$$

and also that

$$\sum_\alpha \frac{\langle \psi \,|\, K_\alpha^\dagger H K_\alpha \,|\, \psi \rangle^2}{w_\alpha} = \\ \sum_\alpha \frac{1}{w_\alpha} \langle \psi \,|\, K_\alpha^\dagger K_\alpha H \,|\, \psi \rangle + 2 \sum_\alpha \delta_\alpha \langle \psi \,|\, K_\alpha^\dagger K_\alpha H \,|\, \psi \rangle + \sum_\alpha w_\alpha \delta_\alpha^2, \tag{B.7}$$

where we have used that $\sum K_\alpha^\dagger K_\alpha = \mathbb{I}$. Hence, we obtain

$$\sum_\alpha w_\alpha V(|\phi\rangle_\alpha) = 4 \left(\langle \psi \,|\, H^2 \,|\, \psi \rangle - \sum_\alpha \frac{\langle \psi \,|\, K_\alpha^\dagger K_\alpha H \,|\, \psi \rangle^2}{w_\alpha} \right). \tag{B.8}$$

Consider now $x_\alpha \equiv \left\langle \psi \,\middle|\, K_\alpha^\dagger K_\alpha H \,\middle|\, \psi \right\rangle$. By invoking the Cauchy-Schwartz inequality, we have

$$\sum_\alpha \frac{x_\alpha^2}{w_\alpha} = \sum_\alpha \frac{x_\alpha^2}{w_\alpha} \sum_{\alpha'} w_{\alpha'} \geq \left(\sum_\alpha \frac{x_\alpha}{\sqrt{w_\alpha}} \sqrt{w_\alpha} \right)^2 = \left(\sum_\alpha x_\alpha \right)^2 = \langle \psi \,|\, H \,|\, \psi \rangle^2 , \tag{B.9}$$

where we have used that $\sum K_\alpha^\dagger K_\alpha = \mathbb{I}$ again in the last step.

In this way, we finally obtain

$$\sum_\alpha w_\alpha V(|\phi\rangle_\alpha) = 4(\left\langle \psi \,\middle|\, H^2 \,\middle|\, \psi \right\rangle - \langle \psi \,|\, H \,|\, \psi \rangle^2) = V(|\psi\rangle). \tag{B.10}$$

Therefore, this proves that the variance of H is non-increasing on average under the measurement $\mathcal{E}$, which implies that conditions (ii) is satisfied. The condition (v) is also satisfied, since

$$V\left(\frac{|e_i\rangle + |e_j\rangle}{\sqrt{2}} \right) = \frac{1}{4} \left(e_i - e_j \right)^2 .$$

Now, we will use the fact that any quantum state ρ can be decomposed in many ways as a mixture of pure states:

$$\rho = \sum_\mu p_\mu \left| \psi_\mu \right\rangle \left\langle \psi_\mu \right| , \tag{B.11}$$

where p_μ are the different probabilities. In the decomposition above, $|\psi_\mu\rangle$ do not necessarily form an orthonormal basis.. Therefore, a *convex roof construction* to extend any real-valued function f of pure states to mixed states:

$$f_{CR} \equiv \inf_{\{p_\mu, |\psi_\mu\rangle\}} \sum_\mu p_\mu \left| \psi_\mu \right\rangle \left\langle \psi_\mu \right| , \tag{B.12}$$

with the optimization over all possible decompositions. One can note that this reduces to f for pure states. It was shown in Ref. [Toloui et al., 2011] that the convex roof of any pure state fulfiling (i)-(iii) is a monotone in all states. Given that in Ref. [Tóth and Petz, 2013] it was shown that

$\mathcal{F}_Q(\rho, H)$ is the convex roof of $V(\psi)$, it follows then that $\mathcal{F}_Q(\rho, H)$ also fulfils the condition (ii).

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