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Frank Eduardo da Silva Steinhoff

Nonclassicality and entanglement

Não-classicalidade e emaranhamento

Campinas, São Paulo - 2013

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Universidade Estadual de Campinas
Instituto de Física Gleb Wataghin

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Abstract / Resumo

Abstract

The present thesis is a collection of results concerning nonclassicality and entanglement, which are fundamental concepts in contemporary quantum physics. We start developing a quasiprobability representation for discrete systems based on sets of mutually unbiased basis, which is a construction related to one pillar of quantum theory: the complementarity principle. The set of classical states in our quasiprobability representation is already present in many related scenarios, both from foundational as well as practical approaches and the notion of classicality obtained is thus well-justified. A deep result follows from our representation: for qubits, the basic units of quantum information theory, the complementarity principle forbids the presence of conjectured configurations beyond quantum physics. Hence, the existence of such superquantum objects would imply a violation of complementarity, a violation that would demand a total reformulation of the conceptual foundations of quantum physics. We present then another result concerning the detection of nonclassicality in terms of observable quantities available in practice. The method is related to the nonclassicality notion induced by the task of entanglement creation, imposing a simple but general definition of classicality for arbitrary physical systems. Finally, we present a novel class of bound entanglement, a non-intuitive phenomenon in entanglement theory that is very hard to characterize. The theoretical construction is based on schemes used currently in quantum optical experiments, thus opening a possibility of practical implementation of bound entangled states in continuous variables systems.

Resumo

A presente tese é um conjunto de resultados relativos à não-classicalidade e ao emaranhamento, que são conceitos fundamentais da física quântica contemporânea. Começamos desenvolvendo uma representação de quasiprobabilidade para sistemas discretos baseada em conjuntos de bases mutuamente não-viesadas, que é uma construção relacionada a um pilar da teoria quântica: o princípio de complementaridade. O conjunto de estados clássicos em nossa representação de quasiprobabilidade já está presente em muitos cenários relacionados, tanto de abordagens fundamentais, bem como práticas e a noção de classicalidade obtida é, portanto, bem-justificada. Um resultado profundo resulta de nossa representação: para qubits, as unidades básicas da teoria da informação quântica, o princípio de complementaridade proíbe a presença de conjecturadas configurações além da física quântica. Assim, a existência de tais objetos superquânticos implicaria uma violação da complementaridade, uma violação que exigiria uma reformulação total das bases conceituais da física quântica. Apresentamos, em seguida, um outro resultado sobre a detecção de não-classicalidade em termos de quantidades observáveis disponíveis na prática. O método está relacionado à noção de não-classicalidade induzida pela tarefa de criação de emaranhamento, que gera uma definição de classicalidade simples mas geral para sistemas físicos arbitrários. Por fim, apresentamos uma nova classe de emaranhamento não-destilável, um fenômeno não-intuitivo em teoria de emaranhamento de difícil caracterização. A construção teórica é baseada em sistemas atualmente utilizados em experimentos de ótica quântica, abrindo assim a possibilidade de implementação prática dos estados emaranhados não-destiláveis em sistemas de variáveis contínuas.

Contents

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Introduction

The precise differences between quantum and classical phenomena are still today a topic of heated debates. It is evident that quantum mechanics is a very distinct theory in the realm of natural sciences, but to isolate it from classical mechanics does not seem to be an easy task. There is an unavoidable ambiguity in the description of measurements in quantum theory that blurs our definitions and assumptions: the apparatus used for observations of a physical system has to be treated both as a quantum and a classical object [1]. Unfortunately, there is no escape from such an ambiguity. The act of measurement in quantum mechanics involves amplification procedures, irreversible and uncontrollable microscopic effects, disturbances caused by the action of the observer, destruction of the states that we want to know about and the list goes on. A quote from Bohr is fruitful:

> *We must be clear that, when it comes to atoms, language can be used only as poetry. The poet, too, is not nearly so concerned with describing facts as with creating images and establishing mental connections.*

It does not mean that nothing can be known or learned from quantum phenomena, but only that the knowledge in quantum theory is mostly partial and intrinsically non-deterministic.

With these limitations in mind, one can still aim at discriminating what are trully nonclassical effects in quantum theory. We do not see in our everyday life cats that are simultaneously alive and dead [2], nor can we choose tomorrow which street we crossed yesterday [3]. Despite their radical character, such bizarre phenomena are only revealed under very special and controlled experimental circumstances. Thus, a consistent operational theory of the experimental arrangement will give us a good way of describing nonclassical phenomena.

The consistent way of handling any experimental data is by the use of probability theory. The experimentalist in the laboratory repeats the same procedure many times in order to have a good distribution of points and to minimize statistical errors.

In quantum regime, a nice way of observing nonclassical phenomena is to analyse the probability distributions associated to preparations and measurements. Nonclassicality reveals itself in its violation of basic probability laws [4]. We are then led to the use of *quasiprobability representations* to describe nonclassical phenomena, an approach that is very general, sucessfull and is currently being used in many different situations [5]. This kind of representation behaves like an usual probability distribution only for a subset of states, which then behave statistically in accordance to standard probability laws; these states are in this sense understood as classical states in relation to the representation, since one cannot differentiate them from a probability distribution. However, the nonclassical character of quantum mechanics cannot be avoided: any quasiprobability distribution will violate a tenet of probability theory in some states or measurements. The message learned is clear: although some quantum objects behave classically in a certain representation, there is no way to consistently represent all quantum phenomena in a single classical framework.

This deep observation actually does more good than harm, since these strange configurations can be used as resources that outperform the limits of classical physics. Thus, the label *nonclassical* is well deserved. Modern quantum information theory reports each day a big number of varied applications of such resources [6, 7, 8] and their characterization is a topic of increasing interest. One of the main aims of the present thesis is to give our contribution to this characterization.

The nonclassical resource that receives more attention in the literature is quantum entanglement [9]. Entanglement is a phenomenon present in composite quantum systems and it is at the heart of many quantum information protocols. Its full characterization is extremelly hard, but its is possible to obtain novel and meaningfull results through reasonable simplifications. Thus, although the full understanding on how to generate entanglement with an arbitrary interaction possibly will demand many generations of research, elegant schemes for usual interactions in a laboratory can be designed. We give our incremental contribution when analysing the task of entanglement creation, which demands a specific kind of nonclassicality notion. Moreover, we give a contribution to the characterization of entanglement *per se*, when we study the non-intuitive phenomenon of *bound entanglement* in a quantum optical setup. The result has both a mathematical/theoretical and a physical/experimental appeal, suceeding despite a very restrictive set of requirements.

Quantum mechanics is very powerfull in comparison to classical physics, but neverthless has its limits [10]. There are classes of problems that even a quantum computer cannot solve efficiently [11]. Interestingly, theories beyond quantum physics break these bounds [12, 13] and have the power to solve any problem requiring ridiculously few resources [14]. Whether such constructions are only a theoretical abstraction or a real phenomenom present in nature is a topic of intense debate nowadays. In this direction, we give our most important contribution in this thesis: for qubits, which are the basic units of quantum information theory, any configuration beyond quantum physics violates the complementarity principle. This significant result is achieved through the development of a new quasiprobability representation, which is related to the complementary aspects of a physical system. Hence, either standard quantum mechanics is indeed the most nonclassical paradigm of nature, with limitations that one should accept, or there is an even weirder paradigm, one that defies our means of consistently defining objective properties.

The thesis is structured as follows:

- In Chapter 1, the fundamental concepts, theorems and definitions needed in further chapters are presented. Concepts which are building blocks of nonclassicality studies - coherent states and phase-space - are presented in a more mathematical fashion, which we try to balance with the physical motivations behind them. We proceed to present operational formulations of the complementarity principle, which is a central topic in the thesis. Then we give a brief review of quantum operations, focusing on the formulations for composite systems, the framework where quantum entanglement will be analysed. Finally, we quickly explain more modern topics such as ontological models, contextuality and superquantum nonlocality. These names are perhaps intimidating for the outsider, but we try to present just the main ideas and concepts involved, without a deep analysis of the details; the interested reader can consult the specialized references cited in the text.

- In Chapter 2, nonclassicality is first presented in terms of quasiprobability distributions, a very powerfull approach that gives a general picture of phenomena beyond classical theories. The quasiprobability representations more related to our work are reviewed and then we present our proposal of quasiprobability distribution based on complementary aspects of discrete systems. The set of classical states associated to the representation appears in many works that give support to our formulation. We then use this construction to show the important conclusion that either the complementarity principle is right, or phenomena beyond quantum physics exist in nature. This is done by carefull analysis of the different assumptions involved. We finish the chapter giving a general method of nonclassicality detection based on the observable quantities that are available in practice. This is done by introducing a simple and general definition of nonclassicality, which is later shown to be related to the task of entanglement creation.

- In Chapter 3, we consider the nonclassical phenomenon known as entanglement, which is the most important concept in quantum information theory. The relevant definitions are quickly seen and then we explain the main separability criteria related to our results. The main ideas in our approach to the task of entanglement creation are shown and the relations to the notion of nonclassicality developed in the previous chapter is presented. Then we proceed to the challenging problem of bound entanglement, describing the main concepts, definitions, results and implications of this special kind of entanglement. The theoretical construction of a new class of bound entagled states is presented, with a somewhat more complex mathematical framework. Then our experimental proposal is described, after comparison with the few previous experiments on bound entanglement implementation. The physical process behind our proposal is a deGaussification in terms of a modified photon-addition. This enables us to overcome the many limitations of other approaches.

- Finally, we give our concluding remarks and point out perspectives of future developments.

Chapter 1

Fundamentals

"The limits of my language are the limits of my world."
Ludwig Wittgenstein

In this chapter it is given a brief review of the topics which are fundamental for this thesis. Some knowledge of elementary group theory[1], matrix analysis [18] and convex analysis[19] is desirable, but we provide quick presentation of concepts when needed and the reader can also consult the specialized books and review articles cited along the thesis for more information.

1.1 Symmetries, stabilizers and coherent states

A symmetry is an operation which leaves invariant some object of interest. For example, after a rotation a ball is still a ball and we say that this object is symmetric under the operation of rotation. This is not its only symmetry: we could reflect all points through the origin and still see the same ball. Indeed, all symmetries of a ball are compositions of reflections and rotations. In physics, identification of the symmetries of physical entities is very valuable, often simplifying difficult problems. Or, in the words of Nobel laureate Phillip Anderson, "physics *is* the study of symmetries" [20].

Mathematically, a symmetry operation is a member of a group. Rotations in three dimensions, for example, form the $SO(3)$ group. In some way all the classical groups - unitary, symplectic, lorentzian - have a great role in quantum mechanics. Of particular importance are the groups associated to the operations and measurements

[1] An introductory book on group theory for physicists is [15]. A more advanced reference is the first chpater of [16]. We will focus on standard results from Lie groups and algebras and a very good introductory text is [17], which also lists the main references on the theme.

performed in a physical system. If the system's Hamiltonian has some symmetry, this will be manifested on the temporal evolution of the states. Also, states and measurements that do not share the symmetry of a physical system can be used as physical resources in certain scenarios, as explained ahead. In quantum mechanics, given a group G, a usefull subgroup is the stabilizer of a state $|\psi\rangle$, given by $G_{|\psi\rangle} = \{g \in G : g|\psi\rangle = \mu(g)|\psi\rangle\}$, where $\mu(g)$ is a scalar. The name says it all: the stabilizer of a state is formed by the operations that leaves this state invariant. Although not explicit in this thesis, important subsets are cosets and normal subgroups, since they give the equivalence classes of the operations performed on a system and thus their classification.

Associated to a symmetry group there exists coherent states, which are those stabilized by the group. Due to historical reasons, coherent states are usually associated to quantum optics; these will be called Canonical Coherent States (CCS) in what follows, while those related to other physical systems will be called Generalized Coherent States (GCS).

Canonical coherent states

In quantum optics, measurements and operations are usually performed through absorption and addition of light quanta. These operations are described as functions of the creation and annihilation operators[2]. The action of the annihilation and creation operator in Fock basis is given respectivelly by

$$a|n\rangle = \sqrt{n}|n-1\rangle; \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{1.1}$$

The Canonical Coherent States (CCS) are by definition the eigenstates of the annihilation operator a: $a|\alpha\rangle = \alpha|\alpha\rangle$, where α is a complex number. Thus, coherent states[3] are those stable under the process of energy absorption. An equivalent definition is given by expressing an arbitrary coherent state as a displacement of the vaccum state,

$$|\alpha\rangle = D(\alpha)|0\rangle \tag{1.2}$$

[2] We are assuming here that the process of absorption/addition of each quantum of light is described by the operator a. This is a good approximation under certain assumptions, but a more general treatment requires that this description should be made by diverse types of operators. See [170] for comments and references on this point.

[3] These states were first introduced by Schrödinger [24], in an analysis of solutions of his equation. The connection with group theory was developed by Klauder [25], while the uses in quantum optics were developed by Glauber and Sudarshan [26, 27].

where the displacement operator is given by

$$D(\alpha) = e^{\alpha a^\dagger - \alpha^* a} \tag{1.3}$$

This way of defining CCS is the most usefull for us, as will be evident in further sections. The expression of a coherent state in Fock basis is simply

$$|\alpha\rangle = e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{1.4}$$

The set of coherent states is an overcomplete basis for the infinite-dimensional Hilbert space, with the following resolution of the identity

$$\frac{1}{\pi} \int_{-\infty}^{+\infty} |\alpha\rangle\langle\alpha| d^2\alpha = I \tag{1.5}$$

This is highly important, since we can express arbitrary operators uniquely as distributions in terms of coherent states. Also, relation (1.5) shows that the coherent states form a POVM (explained further in the text), which is a property that can be explored in many ways.

The normal ordering plays an important role here. A function of the creation and anihillation operators in normal ordering obeys the relation

$$\langle\alpha| f^{(N)}(a^\dagger, a) |\alpha\rangle = f^{(N)}(\alpha^*, \alpha) \tag{1.6}$$

Thus, distributions over the complex plane have a direct correspondence with operators in normal ordering and vice-versa. This will be the basis of the phase-space representation discussed in the next section. A summary of important properties of coherent states:

- Overcomplete resolution of identity given by (1.5);
- One-to-one correspondence between coherent states and points in a classical phase space;
- Functional consistency relation (1.6);
- Minimal uncertainty in measurements of position and momentum.

The last property is easily checked by computing the uncertainty in position and momentum, giving $\Delta q \Delta p = 1/2$, thus achieving the minimum value for Heisenberg's uncertainty relation. This property, however, is not sufficient to characterize a coherent state, since in general a pure state reaches this minimal value if and only if it is Gaussian.

Generalized coherent states and stabilizers

Many attempts to generalize the CCS properties to arbitrary physical systems were proposed, focusing some specific trait of these states. A very elegant and powerfull extension of the formalism can be achieved using the mathematical framework of group theory. Thus, what we call Generalized Coherent States (GCS) here refers to what is known as Group Coherent States in some references. Our treatment is based on [21, 22, 23, 19].

As explained previously, a CCS can be seen as a displacement of the vaccum state

$$|\alpha\rangle = D(\alpha)|0\rangle \tag{1.7}$$

The set of all displacement operators is a Lie-group known as the Heisenberg-Weyl (HW) group, under the product rule $D(\alpha)D(\alpha') = e^{i\phi}D(\alpha+\alpha')$, with $\phi = Im(\alpha\alpha'^*)$. The corresponding (complexified) Lie-algebra is determined by $[a, a^\dagger] = I$. The set of CCS is then the HW-orbit of the vaccum state, which means, roughly speaking, that we apply on the vaccum the elements of the HW group - displacements - to form the whole set of coherent states. In the same vein, given a group G, the set of GCS is defined as the G-orbit of some reference state, choosen by symmetry and/or physical reasons. It is customary to impose some restriction on G, for consistency. A nice way is to demand that G be a Lie-group, so that it is both a group and a manifold. It also captures the dynamic association $U = e^{-iHt/\hbar}$, which is, loosely speaking, related to the connection between the Lie-group of unitaries and the Lie-algebra g of generators. Indeed, if the Hamiltonian of the system is a linear function of the generators in g, a coherent state will evolve to another coherent state. It is also good to demand more structure on G; it is common to consider semisimple Lie-groups, since their classification and structure are tractable. An equivalent definition of a coherent state can be reached through the notion of stabilizers, which are sets defined by

$$G_{|\psi\rangle} = \{g \in G : g|\psi\rangle = \mu(g)|\psi\rangle\}; \tag{1.8}$$

$$\mathsf{g}_{|\psi\rangle} = \{X \in \mathsf{g} : X|\psi\rangle = \lambda(X)|\psi\rangle\} \tag{1.9}$$

where $\mu(g)$ and $\lambda(X)$ are scalars. Pure GCS are those for which the decomposition

$$\mathsf{g} = \mathsf{g}^C_{|\psi\rangle} + \mathsf{g}^{\dagger C}_{|\psi\rangle} \tag{1.10}$$

holds [23], where the superscript C amounts for the complexification[4] of the algebra.

[4]Seeing the algebra as a real vector space and then performing the complexification of this vector

Let us consider the example of $SU(2)$ symmetry[5]. This situation happens often in physical systems like Bose-Einstein condensates, ion-traps, systems composed of spin-1/2 particles and quantum optics. The system not necessarily has this symmetry; in some cases, the interactions or measurements have a good description in terms of elements of $\mathsf{su}(2)$ and the identification and comparison of symmetry-asymmetry is worthwhile. In the case of a great number of spin-1/2 particles, for example, it becomes extremelly hard to estimate the properties of individual particles and what can be actually done is the estimation of collective measurements of angular-momentum operators $\mathbf{J}\cdot\mathbf{n}$, which are elements of $\mathsf{su}(2)$. In the case of Bose-Einstein condensates, it is very profitable to map a double-well into an artificial single angular-momentum system through Schwinger correspondence $j=(n_1+n_2)/2$, $m=(n_1-n_2)/2$, where n_1 (n_2) is the number of particles in the first (second) well.

The underlying Hilbert space of dimension $d=2j+1$ is spanned by $\{|j,m\rangle\}$, where $m=-j,-j+1,\ldots,j-1,j$. The elements of the $\mathsf{su}(2)$ algebra are those satisfying $[J_m,J_n]=i\hbar\epsilon_{mnk}J_k$, where ϵ_{mnk} is the three-dimensional Levi-civita symbol. Thus, $U(s)=e^{i\hbar J_k s}$ is an element of $SU(2)$. We need, however, to parametrize the elements of $SU(2)$ in terms of a complex parameter z, in the same way as the displacement operator in the HW case and also elect an extremal state analogous to the vaccum state. Since the group is semisimple, we choose the maximum weight vector $|j,j\rangle$; to not bore the reader, we give the displacement operator

$$D(z)=(1+|z|^2)^{-j}e^{zJ_-}, \tag{1.11}$$

where J_- is the lowering operator. Then the $SU(2)$ coherent state is simply

$$|z\rangle=D(z)|j,j\rangle=\frac{1}{(1+|z|^2)^j}\sum_{m=-j}^{j}z^k\sqrt{\binom{2j}{j+m}}|j,m\rangle \tag{1.12}$$

The $SU(2)$-orbit is thus $SU(2)/U(1)=\mathbf{S}^2$, the well-known Bloch sphere[6]. The resolu-

space. Since the bracket operation [,] is uniquely extended to the complexified vector space, we have a unique correspondence with a complex algebra [17]. It is important to take this step, since states and operations in quantum theory are supported on complex Hilbert spaces.

[5]This is related to rotational symmetry of a system, i.e., the group $SO(3)$ of rotations in three-dimensions. The problem of using the $SO(3)$ group is that it is not simply-connected. Then the usual procedure is to take its universal covering group, which is $SU(2)$. By the definition of an universal cover [17], $SU(2)$ is a simply-connected group.

[6]It is wise to add the point in infinite, which is the south pole $|j,-j\rangle$ for this orbit; the same is done in every orbit. This is a compactification technique known as one-point compactification, due to Alexandrov [28, 29]. The smart reader will identify the structure of complex projective spaces here; a nice reference in this direction is [19].

tion of identity is ($z = re^{i\phi}$)

$$\frac{2j+1}{4\pi}\int |z\rangle\langle z|d\Omega = \frac{2j+1}{4\pi}\int_0^\infty\int_0^{2\pi}\frac{4r}{1+r^2}|z\rangle\langle z|drd\phi = I \tag{1.13}$$

It is also possible to prove the following uncertainty relation for the $SU(2)$ symmetry:

$$j \leq \Delta^2 \leq j(j+1) \tag{1.14}$$

where $\Delta^2 \equiv \sum_{i=x,y,z}\langle J_i^2\rangle - \langle J_i\rangle^2$, i.e., the variance associated to the Casimir operator $J_x^2 + J_y^2 + J_z^2$. The lower and upper bound are saturated by some $SU(2)$ coherent states. Hence, this kind of coherent states share many features displayed by CCS.

We can also consider G as a discrete group, but the analogies are somewhat loose. We will restrict the discussion here to two discrete groups: the discrete HW group and the Clifford group. Let $\mathcal{H}_d$ be a system of dimension d, with computational basis given by $\{|x\rangle\}_{x=0}^{d-1}$ and let us define the following operators:

$$X|x\rangle = |x \oplus_d 1\rangle \tag{1.15}$$

$$Z|x\rangle = \omega|x\rangle \tag{1.16}$$

where $\omega = e^{i(2\pi/d)}$ is the dth primitive root of unity and $\oplus_d$ is summation modulo d. From this we can generate the following displacement operator

$$T(a_1, a_2) = \omega^{-a_1a_2/2}Z^{a_1}X^{a_2}, \quad (a_1, a_2) \in Z_d \times Z_d \tag{1.17}$$

which is a member of the discrete HW group through the group multiplication rule $T(a_1, a_2)T(a_1', a_2') = e^{i\phi}T(a_1 + a_1', a_2 + a_2')$. A closely related group is the Clifford group of operations, which leave invariant the collection of eigenstates of the various $T(a_i, a_j)$; usually the reference state is the $|0\rangle$ state; the various eigenstates of $T(a_i, a_j)$ are elements of the orbit of the Clifford group. In this sense, they can be regarded as GCS, although this interpretation is not found in the literature.

1.2 Phase space

Historically, most discussions about classicality are based on the phase-space picture of quantum mechanics, due to direct correspondence between classical processes and quantum operations and also due to the powerfull mathematical techniques. Such kind of representation tries to picture states as distributions over an artificial configuration space and usual classical processes as translations, rotations, squeezing and so on are translated as quantum operations through correct quantization of the dynamical variables. The coherent states discussed in the previous section are the building blocks of any such representation.

1.2.1 Continuous representations

For a continuous variable system, it is common to perform a quantization of the classical generalized coordinates q and p, through the association between the Poisson bracket $\{\ ,\ \}$ and the commutator $[\ ,\ ]$

$$\{q, p\} = 1 \rightarrow [Q, P] = iI \tag{1.18}$$

($\hbar = 1$) thus enabling a quantum analog of the classical configuration space. It is common also in quantum optics and quantum field theory to perform the following change of coordinates,

$$a^\dagger = \frac{Q - iP}{\sqrt{2}}; \quad a = \frac{Q + iP}{\sqrt{2}} \tag{1.19}$$

so that the phase-space can be pictured in the complex plane. Since $a|\alpha\rangle = \alpha|\alpha\rangle$, we can represent distributions of the operators a and $a^\dagger$ as distributions of a complex variable α, where the real (imaginary) part of α corresponds to the generalized position (momentum). Also, operations on the distributions are readilly translated in the phase-space. For example, the displacement operator $|\alpha\rangle = D(\alpha)|0\rangle$ and the phase-shifting operator $U(\theta)|\alpha\rangle = |\alpha e^{i\theta}\rangle$ perform translations and rotations. In this context of CCS, an important class of operations are those given by the elements of the symplectic group $Sp(2, R)$, which is the group that preserves the relation $[Q, P] = iI$. These operations have a major role in the study of Gaussian states and Gaussian operations. Gaussian states are completely described by the first and second moments of the creation and annihilation operators. More precisely, all higher order moments of a Gaussian state are functions of the first and second moments, a huge theoretical simplification. Gaussian operations are operations that preserve the gaussianity of a state. These operations are the most easily implementable in an optical experiment and also can be elegantly described through metaplectic representations[7], which connect the operations performed in the laboratory with the symplectic operations appearing in the phase-space picture.

In the broader situation of GCS, there are very general methods of constructing a phase-space representation. If the dynamical symmetry group is semisimple and compact, there is a highest-weight vector which is taken as the reference state. In this case, the G-orbit of this reference state is a Kähler manifold[8], which has always

[7] More on Gaussian states and operations can be checked in [30, 31].

[8] A Kähler manifold is a manifold that is mtutually compatible with three structures: a complex structure, a Riemmannian structure and a symplectic structure [19]

complex, Riemannian and symplectic forms and thus the geometrical structure is in principle straightforward. A nice feature is that the symplectic operations will preserve the form [,] and hence the Lie-algebra of generators of the symmetry group. More than that, we can make the dequantization association between observables M_i in the Lie-algebra[9] and the classical quantities m_i

$$[M_a, M_b] = \sum_c f_{abc} M_c \to \{\langle m_a \rangle, \langle m_b \rangle\} = \sum_c f_{abc} \langle m_c \rangle \tag{1.20}$$

for the states on the orbit of the reference state, which is a precise way of fulfilling the correspondence principle. Indeed, for GCS we have an equivalence between the usual limiting procedures $\hbar \to 0$ and the thermodynamical limit $N \to \infty$ [21](with N being the number of particles).

1.2.2 Discrete representations

In many situations it is fruitiful to have a discretized version of the phase space. We will follow the treatment given by [32] and restrict the discussion to finite dimensions, although the results can be extended to infinite-dimensional systems as well through proper boundary conditions and limiting procedures. For a d-dimensional system, we take a particular orthonormal basis $\{|q_0\rangle, |q_1\rangle, \ldots, |q_{d-1}\rangle\}$ as our position basis; then we have the relations

$$\langle q_i | q_j \rangle \overset{mod\ d}{=} \delta_{i,j}; \qquad \sum_{m=0}^{d-1} |q_m\rangle\langle q_m| = I \tag{1.21}$$

All the operations are made modulo d, unless stated otherwise. We define next the *Finite Fourier Transform*:

$$F = d^{-1/2} \sum_{m,n=0}^{d-1} \omega^{mn} |q_m\rangle\langle q_n|, \tag{1.22}$$

where $\omega = e^{i(2\pi/d)}$ is the d-th rooth of unity - $\omega^0 + \omega^1 + \ldots + \omega^{d-1} = 0$. This transformation has important applications in many quantum algorithms [6]. Next comes the natural definition of momentum states

$$|p_i\rangle = F|q_i\rangle = d^{-1/2} \sum_{j=0}^{d-1} \omega^{ij} |q_j\rangle \tag{1.23}$$

[9]The scalars f_{abc} are known as *structure constants* and determine completely the Lie-algebra [17].

which of course forms another orthonormal basis for the system. We define now position and momentum operators by

$$Q = \sum_{n=0}^{d-1} n|q_n\rangle\langle q_n|; \qquad P = \sum_{n=0}^{d-1} n|p_n\rangle\langle p_n| \tag{1.24}$$

which satisfy clearly the relations $FXF^\dagger = P$ and $FPF^\dagger = -X$. In order to define displacements in phase space, we define the operators

$$Z = e^{i(2\pi/d)Q}; \qquad X = e^{-i(2\pi/d)P} \tag{1.25}$$

As usual, the momentum operator will be the generator of translations in the position basis, made with the operator X and the position operator will be the generator of translations in the momentum basis, made with the operator Z:

$$X^k|q_i\rangle = |q_{i+k}\rangle; \qquad Z^k|p_i\rangle = |p_{i+k}\rangle \tag{1.26}$$

These operators satisfy the relations

$$X^d = Z^d = I; \qquad X^b Z^a = \omega^{-ab} Z^a X^b \tag{1.27}$$

They are also algebraically complete in the sense that any other operator can be expressed as functions of X and Z [33]. In order to see this, let us first show that position and momentum states can be seen as the familiar delta functions:

$$\delta_{Z,k} = |q_k\rangle\langle q_k| = \frac{1}{d}\sum_{m=0}^{d-1}(\omega^{-k}Z)^m; \tag{1.28}$$

$$\delta_{X,k} = |p_k\rangle\langle p_k| = \frac{1}{d}\sum_{m=0}^{d-1}(\omega^{-k}X)^m \tag{1.29}$$

Hence, one can expand any operator F as a function of X and Z:

$$F = \sum_{m,n=0}^{d-1} |p_m\rangle\langle p_m|F|q_n\rangle\langle q_n| = \sum_{m,n=0}^{d-1} \delta_{X,m} f_{m,n} \delta_{P,n} \tag{1.30}$$

with $f_{m.n} = \frac{\langle p_m|F|q_n\rangle}{\langle p_m|q_n\rangle}$. We see also that the phase-space has a toroidal structure; for example, $X|q_{d-1}\rangle = |q_0\rangle$. We now define the displacement operator in phase-space:

$$T(a,b) = Z^a X^b \omega^{-ab/2}; \qquad [T(a,b)]^\dagger = T(-a,-b) \tag{1.31}$$

The discrete HW group multiplication rule is then

$$T(a,b)T(a',b') = \omega^\phi T(a+a', b+b') \tag{1.32}$$

where $\phi = 2^{-1}(ab' - a'b)$.

Symplectic transformations

In the discrete case, a symplectic transformation S preserves the relations (1.27)

$$X' = SXS^\dagger \;=\; X^\kappa Z^\lambda \omega^{-2^{-1}\kappa\lambda} = T(\lambda, \kappa); \tag{1.33}$$

$$Z' = SZS^\dagger \;=\; Z^\mu Z^\nu \omega^{-2^{-1}\mu\nu} = T(\mu, \nu) \tag{1.34}$$

$$\kappa\nu \;-\; \lambda\mu \overset{mod\ d}{=} 1 \tag{1.35}$$

and we can use X' and Z' to form new displacement operators, but in different directions. The integers κ, λ, μ, ν above are elements from Z_d; the relevant question here is, given a triplet κ, λ, μ, whether it is possible to invert them so that $\nu = \kappa^{-1}(1+\lambda\mu)$. When $d = p^n$, all non-zero elements in Z_d are invertible and we have a Galois Field, denoted by $GF(p^n)$; thus our phase space is $GF(p^n) \times GF(p^n)$, which is a finite geometry.

1.3 Complementary measurements and mutually unbiased basis

In classical physics, knowing with certainty any set of physical quantities is in principle just a question of precision and accuracy in the measurements performed. We can simultaneously determine, for example, any characteristic of a bullet that just hit a target: the position it left the gun, its velocity, mass, shape and so on. However, in quantum regime this assumption is no longer valid and can lead to contradictions with many experiments. What is observed is that certainty in some measurement of a fixed experimental preparation precludes certainty in measurements of different quantities. Inspired by the uncertainty relations of Heisenberg [34], Bohr introduced in a series of lectures and essays [35] the so-called *principle of complementarity*[10], which establishes that evidence obtained under different experimental arrangements are complementary, in the sense that they cannot be comprehended simultaneously. The very means of acquiring information forbids us of having absolute knowledge or arbitrary precision for some preparation. Every measurement in quantum mechanics is an amplification act, depending on incontrollable and irreversible processes. Also, the interactions needed to observe some phenomenon unavoidably disturb complementary

[10]There is an enormous number of different formulations of complementarity which we will not review here. A clear explanation of the main ideas can be found in the section entlited *Complementarity* in [36]. A very detailed study is presented in [37].

aspects of an experiment and it is not possible to exclude the apparatus from the description of the phenomenon.

The standard example is given by Young's double slit experiment [38], in which it is possible to observe either wave or particle features of a photon, but not both at the same time. In this experiment, a beam of photons is directed towards a wall with two narrow slits and follows to another wall, in which the light pattern is recorded. The beam intensity is made very small, such that just one photon is incident on the first wall in a suited time period. Thus, if one regards a photon as a particle-like entity, it does make sense to look through which slit the photon passed; this is known as the "which-path" information. If, on the other hand, one regards the photon as a wave-like entity, then we should see on the second wall an interference pattern compatible with the wavefront diffraction; there is then some fringe "visibility". What is observed is that whichever way we try to determine the slit through which the photon passed - the which-way information - completely destroys the interference pattern, i.e., the visibility. If we, however, ignore the which-path information, i.e., if we do not place any detection scheme discriminating the slit that the photon choosed, then the interference pattern is restored.

A quantitative statement of complementarity in the double-slit experiment was obtained by different authors, first experimentally [39] and then theoretically [40], without invoking quantum theory - it is then a real test of complementarity as a physical principle. The fringe visibility V is a well-known quantity in optics and in terms of the maximum and minimum interference fringe intensities I_{max}, I_{min}, it is defined as

$$V = \frac{I_{max} - I_{min}}{I_{max} + I_{min}} \tag{1.36}$$

If P_A (P_B) is the probability that the photon passed through slit A (B), then the distinguishability D of which-way information is given by

$$D = |P_A - P_B| \tag{1.37}$$

The following relation is then obtained for these two complementary quantities:

$$D^2 + V^2 \leq 1 \tag{1.38}$$

and is verified experimentally in many different scenarios.

Complementary operators and mutually unbiased bases

The wave-particle duality in a certain sense can be always observed in a physical system. Given some observable M, certainty in its measurement will inevitably forbids certainty of an obsservable $M' = FMF^\dagger$, where F is the Fourier transform of the system, be it discrete or continuous. There are, however, more complementary aspects in a given experiment, in such a way that the collection of all complementary measurements yields a complete statistical description of the system. Complementary measurements are best described by the use of *mutually unbiased bases* (MUB). A recent review on the subject can be found in [33].

Two orthonormal bases of a d-dimensional system $A = \{|a_i\rangle\}_{i=0}^{d-1}$ and $B = \{|b_j\rangle\}_{j=0}^{d-1}$ are mutually unbiased if they satisfy

$$|\langle a_m|b_n\rangle|^2 = 1/d \tag{1.39}$$

for all m, n. To see how complementarity applies, let us define a non-degenerate observable $M = m_0|a_0\rangle\langle a_0| + m_1|a_1\rangle\langle a_1| + \ldots m_{d-1}|a_{d-1}\rangle\langle a_{d-1}|$. If, for example, we prepare the state $\rho = |a_k\rangle\langle a_k|$, the outcomes of M are completelly determined: the outcome m_k occurs with unit probability, $Tr(|a_k\rangle\langle a_k|\rho) = 1$, while the outcomes m_i, for $i \neq k$, never occur: $Tr(|a_i\rangle\langle a_i|\rho) = 0$. Now, if we measure a nondegenerate observable supported on the mutually unbiased base B, i.e., $N = n_0|b_0\rangle\langle b_0| + n_1|b_1\rangle\langle b_1| + \ldots n_{d-1}|b_{d-1}\rangle\langle b_{d-1}|$, each outcome n_k will be completelly random, occuring with probability $1/d$. In this sense, the observables M and N are complementary: certainty in the measurements of one precludes any certainty in the measurements of the other.

There are many algorithms to construct sets of MUB when the dimension of the system is a power of a prime number p, i.e., $d = p^n$. In this situation it is possible to define a finite field, also known as Galois field $GF(p^n)$, a construction already saw in discrete phase space representations. Also, it is proved that there is a maximal number of $d+1$ MUB and thus the measurements on these bases is informationally complete: using $d+1$ complementary measurements with $d-1$ independent outcomes gives $(d-1)(d+1) = d^2 - 1$ independent outcomes, which is the number needed to specify any unknown density matrix of the system. At least one pair of MUB is easy to construct in any dimension: a basis $A = \{|a_i\rangle\}_{i=0}^{d-1}$ and $B = \{F|a_i\rangle\}$ are clearly mutually unbiased. The basis elements are eigenvectors of the operators X and Z. As proved in [42], for $d = p^n$ the eigenvectors of XZ, XZ^2, …, XZ^d form the other $d-1$ MUB needed.

The geometry associated to MUB is very rich. We will follow the work of Appleby [41], where the description of MUB sets is considered in terms of Bloch representations in arbitrary finite dimensions. For a d-dimensional system, an arbitrary state can be expressed in terms of a Bloch vector as

$$\rho = \frac{1}{d}(I + \mathbf{B}) \tag{1.40}$$

where $\mathbf{B}$ is a trace-zero Hermitian matrix in $\mathsf{su}(d)$. Regarding $\mathbf{B}$ as a vector, one can define the inner product with a different vector $\mathbf{B}'$

$$< \mathbf{B}, \mathbf{B}' >= \frac{1}{d(d-1)} Tr(\mathbf{B}\mathbf{B}') \tag{1.41}$$

and the induced norm is $||\mathbf{B}|| =< \mathbf{B}, \mathbf{B} >^{1/2}$. Considering some orthonormal basis $\{|\psi_0\rangle, |\psi_1\rangle, \ldots, |\psi_{d-1}\rangle\}$ we associate to each state the Bloch vectors $\mathbf{B}_i = d|\psi_i\rangle\langle\psi_i| - I$; then we have

$$\sum_{i=0}^{d-1} \mathbf{B}_i = \mathbf{0}; \tag{1.42}$$

$$< \mathbf{B}_i, \mathbf{B}_j > = \frac{1}{d-1}(d\delta_{ij} - 1) \tag{1.43}$$

An orthonormal basis defines then a regular simplex[11] in this Bloch picture. More importantly, the inner product of Bloch vectors $\mathbf{B}_\psi = d|\psi\rangle\langle\psi| - I$, $\mathbf{B}_\phi = d|\phi\rangle\langle\phi| - I$ satisfies $< \mathbf{B}_\psi, \mathbf{B}_\phi >= 0$ if and only if $|\langle\psi|\phi\rangle|^2 = 1/d$, i.e., iff the states are mutually unbiased. Hence, in this picture the simplices of MUB are orthogonal to each other.

Moreover, this approach is closely related with the geometrical structure known as *complementarity polytope* [43]. This is a polytope that is constructed in arbitrary finite-dimensional systems by taking $d+1$ regular simplices, each with d corners at unit distance from each other. The complementarity polytope is the convex hull[12] of the $d(d+1)$ corners of these simplices. In the cases where there exists complete sets of MUB, the convex hull of the $d(d+1)$ states will then correspond to the complementarity polytope; in the situation $d = p^n$, it is known that such complete sets exist. The question on the existence of complete sets of MUB in arbitrary dimensions is then translated geometrically as the problem of rotating the complementarity polytope in such a way that its corners lie inside the Bloch ball of density matrices.

The study of MUB has received an increasing interest in recent years[13]. The problem on the maximal number of MUB in non-prime power dimensions is an old one in mathematics, but it receives different names and meanings depending on the

[11] A p-simplex is the set of all points of the form

$$\mathbf{x} = \lambda_0\mathbf{x}_0 + \lambda_1\mathbf{x}_1 + \ldots + \lambda_p\mathbf{x}_p \tag{1.44}$$

with $\lambda_i \geq 0$ and $\sum_{i=0}^{p} \lambda_i = 1$.

[12] The convex hull of a set of points X is the smallest convex set that contains X. For a set of finite cardinality S, the convex hull coincides with the set of all convex combinations of points in S.

[13] We are thankfull to Prof. Galvão for many references listed in this paragraph and pointing out the connection of our work with the complementarity polytope construction.

approach used [44]. The quantum information formulations started with Wootters and Fields [45], highlighting the minization of statistical errors when using measurements in MUB for the task of state reconstruction. The general geometrical picture and connection with the problem on the existence of SIC-POVMs (explained further in the text) and quantum designs was given by Wootters in [46]. In the mean time, Gottesmann presented the famous *Gottesmann-Knill Theorem* [47], which introduced the stabilizer formalism approach to quantum computation theory through the use of the discrete Wigner function - which will be seen in the next chapter. Later on, the connection between the Gottesmann-Knill (GK) theorem and sets of MUB was found [48], greatly increasing the relevance of the research on MUB. More recently, schemes using complementary quantities associated to MUB were applied to the detection of entanglement [49].

Complementarity/duality relations

The duality relation (1.38) is ideal for tests of complementarity, since it is independent of the quantum formalism and is supported experimentally. We would like similar relations for sets of MUB, since complementarity is so well expressed for these sets. The relations should depend only on the probabilities measured in the laboratory and not depend on the quantum formalism. In a series of works [50], Luis developed general relations of complementarity and duality for discrete systems. The relations are general enough to quantitatively describe complementary aspects of arbitrary collection of observables, but we will focus on the relations derived for complementary measurements in MUB. We give more reasons for this choice further in the text, but a quick justification is that for a fixed set of complementary measurements there are connections to other works on complementarity which do not refer explicitly to quantum theory.

Before considering Luis' relations, let us briefly present alternative approaches based on uncertainty relations. The seminal and most known uncertainty relation is Heisenberg-Robertson Uncertainty Relation [34]. Given observables A and B, the relation reads

$$\Delta_A \Delta_B \geq \frac{1}{2} |\langle [A, B] \rangle| \tag{1.45}$$

where Δ_M is the standard deviation of the measurements of an observable: $\Delta_M = \sqrt{\langle M^2 \rangle - \langle M \rangle^2}$. The standard deviation is not an unbiased estimator in many situations and this fact motivated the development of entropic uncertainty relations by different authors [51], since entropy does not suffer from such problem and also there are more possibilities of interpretation in terms of information and disorder of a system. A very complete review on the subject can be found in [52]. For our discussion, the important relation is

$$H_{B_1} + H_{B_2} \geq \log d \tag{1.46}$$

where H_{B_1} and H_{B_2} are respectivelly the entropies of measurements[14] in the MUB B_1 and B_2. It is easy to see that the lower bound is reached precisely in the elements of the MUB. Although being general, uncertainty relations are somewhat dependant on the mathematical framework of quantum mechanics; one cannot talk about uncertainties without invoking Born's rule, hermitean operators, commutators and so on. While uncertainty relations indicate limitations on the precision of measurements, complementarity indicate the limitations on the definitions we can make about physical quantities [37]. Thus, we now turn to the more general framework of complementarity (but returning to uncertainty relations once in a while).

Let $P_M(m)$ be the probability of obtaining outcome $m = 0, 1, \ldots, M-1$ when measuring the observable M. The characteristic function associated to this probability distribution is

$$C_M(\tilde{m}) = \sum_{m=0}^{M-1} e^{i2\pi m\tilde{m}/M} P_M(m) \tag{1.47}$$

where $\tilde{m} = 0, 1, \ldots, M-1$. The modulus of the characteristic function above can be regarded as a degree of certainty one can have about the value of the quantity M: when $P_M(m) = \delta(m, m_0)$, we have a maximal certainty $|C_M(\tilde{m})| = 1$, while when $P_M(m) = 1/M$, we have $|C_M(\tilde{m})| = 0$, for all $\tilde{m} \neq 0$. Let us define the certainty of this distribution as

$$C_M^2 = \frac{1}{M} \sum_{m=0}^{M-1} |C_M(\tilde{m})|^2 \tag{1.48}$$

Then it is easy to verify that

$$C_M^2 = \sum_{m=0}^{d-1} P_M^2(m) \tag{1.49}$$

Let us consider a certain number of complementary observables M_j, $j = 1, \ldots, J$, made of N orthogonal projectors. Then it is possible to prove the following relations for any

[14] More precisely, the Shannon entropies of the outcomes' probabilities: $H_B = -\sum_i p_i \log p_i$, where $B = \{|\psi_0\rangle, |\psi_1\rangle, \ldots, |\psi_{d-1}\rangle\}$ is some orthonormal basis where we perform measurements whose outcomes occur with probabilities $p_i = \langle\psi_i|\rho|\psi_i\rangle$.

dimension N:

$$\sum_{j=1}^{J} C_j^2 \leq 1 + \frac{J-1}{\sqrt{N}} \tag{1.50}$$

$$\prod_{j=1}^{J} C_j \leq \left[\frac{1}{J}\left(1 + \frac{J-1}{\sqrt{N}}\right)\right]^{J/2} \tag{1.51}$$

When N is a power of prime, then we have the stronger relation:

$$\sum_{j=1}^{J} C_j^2 \leq 1 + \frac{J-1}{N} \tag{1.52}$$

Moreover, measuring the full spectrum of complementary observables - $J = N+1$ - we arrive at the relation

$$\sum_{j=1}^{N+1} C_j^2 \leq 2 \tag{1.53}$$

which will be used in many occasions in further sections. These will be the complementary relations we will refer to. These relations can be derived independently from quantum theory, just assuming simple probability theory. Also, even considering negative values of probability one can reason in terms of complementarity, which is a major advantage.

The qubit case

Let us illustrate the ideas of complementarity in a bidimensional system, also refered as a qubit. The root of unity here is simply $\omega = e^{i\pi} = -1$ and the $2+1 = 3$ MUB are those constituted by eigenvectors of the Pauli matrices, which in the computational basis $\{|0\rangle, |1\rangle\}$ are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.54}$$

with respective eigenstates

$$|x_\pm\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \pm |1\rangle\right); \tag{1.55}$$

$$|y_\pm\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \pm i|1\rangle\right); \tag{1.56}$$

$$|z_+\rangle = |0\rangle; \quad |z_-\rangle = |1\rangle \tag{1.57}$$

The MUB set associated to the computational basis is then $\mathcal{B}_i = \{|i_+\rangle, |i_-\rangle\}$, for $i = x, y, z$. Notice that vectors in each basis satisfy the relation

$$|\langle\phi_i|\phi_j\rangle|^2 = \frac{1}{2} \tag{1.58}$$

Let us see the geometrical relations in terms of Bloch vectors. We see that $\mathbf{B}_i^{(\pm)} = 2|i_\pm\rangle\langle i_\pm| - I$ give the three Pauli matrices with plus or minus sign. The simplex relation $\mathbf{B}_x^{(+)} + \mathbf{B}_x^{(-)} = 0$, for example, is the trivial relation $\sigma_x + (-\sigma_x) = 0$; for higher dimensions the relations are not so simple.

Higher dimensions

For higher dimensions, if $d = p^n$ for p prime, then the $d+1$ MUB are formed by the eigenstates of X, Z, XZ, XZ^2, $\ldots$, XZ^{d-1}. Let us consider the case of a qutrit ($d = 3$) first. In this situation, we have operators

$$X = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix} \tag{1.59}$$

and the set of MUB is given by

$$\mathcal{B}_i = \{|0^{(i)}\rangle, |1^{(i)}\rangle, |2^{(i)}\rangle\} \tag{1.60}$$

where $i = 1, 2, 3, 4$, $|0^{(1)}\rangle \equiv |0\rangle$, $|1^{(1)}\rangle \equiv |1\rangle$, $|2^{(1)}\rangle \equiv |2\rangle$ and

$$|0^{(2)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + |2\rangle); \tag{1.61}$$

$$|1^{(2)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + \omega|1\rangle + \omega^2|2\rangle); \tag{1.62}$$

$$|2^{(2)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + \omega^2|1\rangle + \omega|2\rangle); \tag{1.63}$$

$$\tag{1.64}$$

$$|0^{(3)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + \omega|1\rangle + \omega|2\rangle); \tag{1.65}$$

$$|1^{(3)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + \omega^2|1\rangle + |2\rangle); \tag{1.66}$$

$$|2^{(3)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + \omega^2|2\rangle); \tag{1.67}$$

$$\tag{1.68}$$

$$|0^{(4)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + \omega^2|1\rangle + \omega^2|2\rangle); \tag{1.69}$$

$$|1^{(4)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + \omega|1\rangle + |2\rangle); \tag{1.70}$$

$$|2^{(4)}\rangle \equiv \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + \omega|2\rangle); \tag{1.71}$$

$$\tag{1.72}$$

where $\omega = e^{2\pi i/3}$. The Bloch vector for each state is then $B_i^{(j)} = 3|i^{(j)}\rangle\langle i^{(j)}| - I$, with $i = 0, 1, 2$ and $j = 1, 2, 3, 4$. The matricial representation in the j-th base is

$$B_0^{(j)} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}; \quad B_1^{(j)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}; \quad B_2^{(j)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}; \tag{1.73}$$

It is straightforward then that $B_0^{(j)} + B_1^{(j)} + B_2^{(j)} = 0$ holds in all bases. The extension to higher prime-power dimensions is straightforward.

1.4 Composite systems: the SLOCC paradigm

As is well-known, a Hilbert space $\mathcal{H} = \bigotimes_i \mathcal{H}_i$ describes a system composed by subsystems $\mathcal{H}_i$. Since states in quantum mechanics are described by positive semidefinite operators, it is important to have a good grasp of linear transformations that preserve positivity of operators, both in the subsystems $\mathcal{H}_i$ as well as in the global system $\mathcal{H}$.

Definition 1 *A map $\Lambda : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}')$ is called positive if for all positive semidefinite $M \in \mathcal{B}(\mathcal{H})$ we have that $\Lambda(M) \in \mathcal{B}(\mathcal{H}')$ is positive semidefinite as well. A positive map is called Completely Positive (CP) if $\Lambda \otimes I_k$ is a positive map for any $k = 0, 1, 2, \ldots$; otherwise the map is Non-Completely Positive (NCP).*

In quantum mechanics, CP maps are used to described any operation that one can perform in a closed quantum system [6], while NCP maps can describe the dynamics of open systems [55] and also have a great role in entanglement theory, as we will see in Chapter 3.

Quantum operations

A quantum operation in an isolated system is given by a linear CP map $\Lambda : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}')$, satisfying $0 \leq Tr[\Lambda(\rho)] \leq 1$. The state after the operation is given by

$$\rho' = \frac{\Lambda(\rho)}{Tr[\Lambda(\rho)]} \tag{1.74}$$

where $Tr[\Lambda(\rho)]$ is the probability of sucess of the operation. The demand for complete positivity can be interpreted physically as a way to guarantee that any composition of a physical system with an ancillary system will not affect the validity of the operation as a physical process.

Any quantum operation Λ admits a Kraus or operator-sum representation [6, 53, 7]

$$\Lambda(\rho) = \sum_k E_k \rho E_k^\dagger \tag{1.75}$$

with $\sum_k E_k E_k^\dagger \leq I$. When the Kraus operators satisfy $\sum_k E_k^\dagger E_k = I$, we say that the operation is deterministic, since $Tr[\Lambda(\rho)] = Tr[\sum_k E_k \rho E_k^\dagger] = Tr[(\sum_k E_k^\dagger E_k)\rho] = 1$; otherwise, the operation is stochastic. It is always possible to see a deterministic operation as a restriction of a unitary operation that acts in an artificial enlarged system. Taking an orthonormal basis $\{|i\rangle\}_{i=0}^{d-1}$ of the original Hilbert system $\mathcal{H}$, we take an orthonormal basis $\{|e_k\rangle\}_{k=0}^{d'-1}$ of an ancillary system $\mathcal{H}'$; in the total system $\mathcal{H} \otimes \mathcal{H}'$, we define the operator

$$U|i\rangle \otimes |e_0\rangle = \sum_k E_k |i\rangle \otimes |e_k\rangle \tag{1.76}$$

It is easy to see that U is indeed unitary:

$$\begin{aligned}
\langle i| \otimes \langle e_0| U^\dagger U |i\rangle \otimes |e_0\rangle &= \left(\sum_{k'} \langle i| \otimes \langle e_k| E_{k'}^\dagger \right) \left(\sum_k E_k |i\rangle \otimes |e_k\rangle \right) && (1.77)\\
&= \sum_k \langle i'| E_k^\dagger E_k |i\rangle && (1.78)\\
&= \langle i'|i\rangle && (1.79)
\end{aligned}$$

It is a simple exercise to show that the converse is also true: a unitary over a composite system in general is a non-unitary quantum operation for the subsystems [6].

Measurements in quantum mechanics are described by the use of a *Positive Operator Valued Measure* (POVM), which is a set of positive operators $\{E_k\}$ such that $\sum_k E_k = I$; an element of this set is called an *effect*. A Projective Value Measure (PVM) is a special case of a POVM, occuring when all effects E_k satisfy $E_k^2 = E_k$ and are orthogonal. Projective measurements (not measures) on coherent states form a POVM by the overcomplete resolution of identity (1.5). The measurements are not orthogonal, since coherent states overlap and this means that the events described by coherent states are not mutually exclusive. POVMs are in this sense a generalization of PVMs, enabling one to construct probability measures from arbitrary resolutions of identity. An important theorem due to Naimark (see Section 9.6 from [1].) shows that any POVM can be seen as a PVM in an enlarged system. Conversely, PVMs in a composite system are described by POVMs in the subsystems.

SLOCC operations

Quantum operations in composite systems[15] can be subject to certain constraints due to possible spatial separations between the subsystems, practical difficulties of transmiting quantum particles or impossibilities of performing certain kinds of measurement. If, for example, the subsystems are separated by a space-like distance then an arbitrary quantum operation must respect the principle of non-signalling. An allowed operation in this case would then be $U_A \otimes U_B$, with U_A and U_B unitaries, while the swap operation $U = \sum_{i,j} |ij\rangle\langle ji|$ would be forbidden, since it would imply an instantaneous exchange of quantum particles, violating non-signaling in this example. In general, joint quantum operations are discarded, given their inacessibility in many practical situations. The parties are allowed, however, to act locally in their own subsystems, to exchange classical information and act in a correlated way conditioned to this information. This is the situation known as the paradigm of *Stochastic Local Operations and Classical Communication* (SLOCC), i.e., the allowed quantum operations are local and intermediated through classical communication and could be also subject to (local) stochastic processes.

The Kraus representation of this class of operations is given by

$$\Lambda_{sep}(\rho) = \sum_k (A_k \otimes B_k)\rho(A_k^\dagger \otimes B_k^\dagger) \tag{1.80}$$

with $\sum_k (A_k^\dagger A_k) \otimes (B_k^\dagger B_k) \leq I$. Operations in the form Λ_{sep} above are termed *separable operations*. As proved in [54], a CP map can be generated by SLOCC iff it can be written in the form Λ_{sep} above. A special class is that formed by operators that satisfy $\sum_k (A_k^\dagger A_k) \otimes (B_k^\dagger B_k) = I$, so that Λ above is deterministic; in this case, we use the name LOCC.

[15] We will restrict the discussion to a bipartite system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, but the extensions to multipartie systems are straightfoward.

1.5 Ontological models and contextuality

An operational theory[16] models mathematically a physical experiment in terms of preparations, measurements, outcomes and systems. These are primitive notions which should somehow be consistently stated, compared with the phenomena observed and interpreted in the light of usual concepts such as probabilities and flow of time. Ambiguities here are unavoidable, given that we are constrained to express our findings in terms of our everyday-life language. For example, what are the distinctions between a preparation and a measurement in a given experiment? A pragmatic approach would state that[17] "a photon *is* the click in a photon detector". Different formulations can even make clear distinctions between the preparation and the state that is used to describe the physical situation. One should try to restrict such interpretative ambiguities to a minimum by the imposition of a robust set of postulates, but it is clear that the clash between different interpretations will never cease.

A preparation is a completely specified experimental procedure; a set of mutuallly exclusive preparations for a experiment forms then a set $\mathcal{P}$. In a experiment, a preparation $P \in \mathcal{P}$ is subjected to a measurement M, which is an element of a set $\mathcal{M}$ of mutually exclusive measurements. This irreversible procedure gives some outcome k, which is one of a set $\mathcal{K}$ of mutually exclusive and exhaustive outcomes. The objective of any operational theory is to determine the probabilities $p(k|P, M)$, i.e., the probability that outcome k occurs given that we are performing the measurement M of the preparation P. The use of probability theory does not mean that the operational theory is intrinsically non-deterministic; deterministic theories are just a special case of the formalism and there are also deterministic regimes inside any operational theory. Summarizing, an operational theory is a specification $\{\mathcal{P}, \mathcal{M}, \mathcal{K}, p(k|P, M)\}$. It is immediate that $\sum_k Pr(k|P, M) = 1$; also, from standard probability theory the following decomposition is straightforward:

$$p(k, \bigvee_i P_i, \bigvee_j M_j) = \sum_{i,j} p(k, P_i, M_j) \tag{1.81}$$

An ontological model of an operational theory is an introduction of an ontic state λ which would describe the outcomes $k \in \mathcal{K}$ independently on the preparation or the measurements performed. In other words, k is independent of P given λ. However, due to some technological inability to know the ontic state λ, we would need to construct an epistemic theory for the probabilities of outcomes, given by our operational theory

[16]This section is based on the review [5] and some concepts of [1].

[17]Quote attributed to Zeilinger [56].

$\{\mathcal{P}, \mathcal{M}, \mathcal{K}, p(k|P, M)\}$. The need to refer to the preparation P would result from the ignorance of λ; we can say, for example, that statistical physics is an epistemic theory resulting from the ignorance of the ontic state describing the system, which is totaly known if the initial state is known.

The independence of λ on the preparation and measurements could leave open the possibility that different preparations or measurements could in principle ascribe different probabilities to the outcomes viewed in an experiment. To avoid this strange possibility, the concept of *non-contextuality* is introduced:

Definition 2 *An ontological model is*

- *Preparation non-contextual if for all* $P, P' \in \mathcal{P}$*,*

$$p(k|P, M) = p(k|P', M) \Rightarrow p(\lambda|P) = p(\lambda|P') \tag{1.82}$$

- *Measurement non-contextual if for all* $M, M' \in \mathcal{M}$*,*

$$p(k|P, M) = p(k|P, M') \Rightarrow p(k|\lambda, M) = p(k|\lambda, M') \tag{1.83}$$

Quantum physics is an operational theory that associates to each preparation P a density matrix ρ_P and to each measurement M with outcome k an effect $E_{M,k}$; this association does not need to be one-to-one. The probability given by quantum theory is given by Born's rule $p(k|P, M) = Tr(\rho_P E_{M,k})$. It is noteworthy that this rule is a consequence of the formulation in terms of a Hilbert space, as discovered by Gleason [57] and Busch [58].

1.6 Nonlocal boxes

Nonlocality seems to be the most radical consequence of quantum mechanics. Even not violating relativity, nonlocal correlations give an uneasy feeling that "spooky" influences between causally disconnected physical systems occur in nature. It is a natural impulse to consider that quantum theory is merelly the result of our ignorance of a real theory governed by some hidden variable which, due to technical limitations, would not be available for us. In this direction, Einstein, Podolsky, Rosen (EPR) [59] attempted to prove that quantum theory was incomplete in its description of physical phenomena. Later on, Bohm [60] reproduced the results of quantum theory by the use of a deterministic *Hidden Variable Theory* (HVT). Although these approaches seem to have failed when confronted with nature, they brought the discussion to a whole new level in the natural sciences.

The Bell-CHSH inequality

The starting point of quantum information theory is the discovery by Bell [62] that it is impossible to reproduce the predictions of quantum mechanics with a deterministic *Local Hidden Variable Theory* (LHVT). A LHVT[18] is based on the following assumptions:

1. *Locality:* Operations performed on a physical system A cannot influence another physical system B, if A and B are separated by a space-like distance, i.e., measurement outcomes at A do not depend on Bâs choice of setting.

2. *Realism:* Properties of a physical system exist prior to their observation. In the Stern-Gerlach experiment, for example, there is no question that the intrinsic-angular momentum (spin) is quantized, since it is an experimental fact that $\pm\hbar/2$ are the only values that are observed in this setup. However, wheter the spin has $+\hbar/2$ or $-\hbar/2$ is already certain prior to the measurement. We are ignorant of this value due to technical reasons; had we access to the hidden variable describing the system, then every future behaviour would be determined. In this sense, quantum rules are seen as having an epistemic origin, rather than being intrinsic properties of nature.

3. *Free will:* We can freely choose the measurements to be performed on a physical system. Freely here means that one can choose among a set of different measurements through a random process and also that the settings at A nad B can be independently chosen.

Later on, Clauser, Horne, Shimony and Holt (CHSH) proved a stronger statement [63]: even a stochastic LHVT theory does not correspond to the outcomes observed in quantum experiments. This means that even if we introduced some randomness on a candidate classical description of a quantum system - e.g., classical chaos, stochastic fluctuations of a classical field, the results of lottery, etc. - this description would not correspond to the observed data by a significant amount. Quantum physics has something more. To prove this, let us consider a bipartite system where (A_1, A_2) are dichotomic variables in the first subsystem and (B_1, B_2) dichotomic variables in the second subsystem. Then one proves that the following inequality

$$|\langle A_1 B_1\rangle + \langle A_1 B_2\rangle + \langle A_2 B_1\rangle - \langle A_2 B_2\rangle| \leq 2 \tag{1.84}$$

[18] We will not review all the assumptions and definitions underlying a description in terms of LHVT, since there is a zoo of articles, books and thesis that already do this. Very good reviews are given in [1, 61] and the reader can consult the references therein.

known as Bell-CHSH inequality, is valid for any LHVT. An important remark is that this result depends solely on elementary probability rules and the assumptions of locality, realism and free-will, not refeering to quantum theory. In the quantum case, to measure this quantity one introduces the operator

$$B = A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2 \tag{1.85}$$

and A_i, B_j are observables with eigenvalues ± 1; the inequality then reads $|\langle B \rangle| \leq 2$. In a bidimensional system, we take the observables $A_1 = -\sigma_x$, $A_2 = -\sigma_y$, $B_1 = (\sigma_x + \sigma_y)/\sqrt{2}$ and $(\sigma_x - \sigma_y)/\sqrt{2}$ and compute the mean value of the operator B for the singlet state $|\phi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$, obtaining $|\langle B \rangle| = 2\sqrt{2}$, which violates the Bell-CHSH inequality, implying that at least one of the assumptions of a candidate LHVT should be wrong. This result demolishes any dream of a local realistic description of the world... assuming, of course, that quantum theory is a faithful description of nature.

Although it may sound strange to test experimentally an algebraic inequality, the Bell-CHSH inequality relies on assumptions that are not that simple to arrange in a laboratory and it is a good idea to measure the correlations and see if everything goes according to the plan. The first experiment to observe the violation of a Bell-CHSH inequality was given by Aspect *et al* [64], where an ingenious method was developed to create the required space-like separation between the subsystems. This experiment fostered a boom in both theoretical and experimental research on quantum nonlocality, which is a current trend up to now. We stress that the subject is far from a resolution, since many types of objections can be raised in experiments on nonlocality.

Quantum contextuality

The original formulation of contextuality was based on the mathematical formalism of quantum theory. Hidden variables models of quantum mechanics often implicitly assume two apparently very reasonable premisses:

1. *Independence on the context*: The measurement outcome of an operator A depends solely on the choice of A and the objectives properties of the system to be measured. In particular, if A commutes with other operators B e C, the outcomes of A do not depend on its context, i.e., the outcomes do not depend on measuring only A, or A and B, or A and C.

2. *Functional consistency*: Given two commuting operators A and B, given an operator function $f(A, B)$, the measurement outcomes of A and B follow the same functional relation of the operators.

Despite their reasonability, these conditions conflict with quantum mechanics; this was first proved by Kochen and Specker [65], in what is now known as the Kochen-Specker (KS) Theorem. A direct consequence [66] is that if there exists operators A, B and C such that $[A, B] = 0$, $[A, C] = 0$, but $[B, C] \neq 0$, we will have that the outcomes of A will depend whether we choose to measure A simultaneously with B or C; in this sense quantum mechanics is contextual.

Superquantum nonlocality

There is an upper limit for the violation of Bell-CHSH inequalities by quantum theory known as *Tsirelson's bound* [10], which forces the following limit on any bipartite quantum state ρ:

$$|\langle B(\rho)\rangle| \leq 2\sqrt{2} \tag{1.86}$$

The source of such bound is discussed in many works, but there is no general consensus on the subject. A different viewpoint was given by Popescu and Rohrlich [12], in a work that assumed nonlocality and no-signalling as the relevant axioms instead of quantum mechanics. The authors showed the existence of nonlocal correlations that did not violate relativity theory, but that violated Tsirelson's bound, reaching a Bell-CHSH value of 4. Thus, there are perfectly legitimate probabilistic theories that are more nonlocal than quantum mechanics and nevertless do not display faster than light signals. Following this discovery, surged the development of theories in terms of *nonlocal boxes* [13], which are theories respecting the no-signalling principle and with a certain amount of nonlocality. The study of such objects is not just a mere curiosity, since their existence would imply a computational power beyond imagination [14].

Chapter 2

Nonclassicality

"Quantum mechanics: real black magic calculus."
Albert Einstein

2.1 Notions of nonclassicality

There are many different understandings on how to define and discriminate the non-classical aspects of quantum states. Two different notions of nonclassicality are usual in the literature:

- *Foundational approach:* It is not possible to consistently interpret all states and operations in quantum theory in terms of classical concepts[1]. Examples include Bell-CHSH theorem [62], Kochen-Specker theorem [65], Gleason's theorem [57] and more recently Spekken's theorem [67, 68].

- *Resource approach:* Some quantum states and operations outperform tasks performed classicaly, being thus nonclassical resources for these tasks. Examples include entanglement, squeezing, teleportation, quantum computing and almost all studies in quantum theory of information.

The foundational approach struggles with the assumptions implicit in the definitions and interpretation of data. In any experiment on Bell inequalities violation, things to look for are the absence of detection loopholes, what is meant by locality for that system, whether the experimentalists were sucessfull in obtaining spacelike separations and so on. The resource approach is much more pragmatic and easier to handle, but in

[1] A recent overview of many foundational approaches can be found in [69].

many situations it is difficult to see from where the advantages come from, or even to verify such an advantage, i.e., to identify the tasks for which quantum states outperform classical ones. There is some struggle, for example, to identify whether computational speed-up really happens in some proposals of quantum technologies[2].

2.2 Quasiprobability distributions

A way of handling the foundational and resource approaches in the same footing is by the use of quasiprobability distributions. These are distributions over the state space which only qualify as genuine probability distributions in some convex subset, violating at least one axiom of probability outside this special subset, which is considered then the set of classical states. The formal definition related to ontological models is then [5]:

Definition 3 *A quasiprobability representation of quantum theory is a pair of affine mappings μ, ξ which satisfy, for every ontic state λ, density matrix ρ and all effect E:*

- $\mu_\rho(\lambda) \in R$ *and* $\sum_\lambda \mu_\rho(\lambda) = 1$;
- $\xi_E(\lambda) \in R$ *and* $\xi_I(\lambda) = 1$;
- $Tr(\rho E) = \sum_\lambda \mu_\rho(\lambda)\xi_E(\lambda)$

The following result is equivalent to Spekkens' Theorem [67, 68]:

Theorem 1 *A quasiprobability representation of quantum theory must have negativity in either its representation of states or measurements (or both).*

The set of positivelly represented states is thus in a one-to-one correspondence to an ontological model, being classically represented. We stress that the requirements imposed by a quasiprobability representation are too strong to capture all notions of nonclassicality. This will be evident when we treat the task of entanglement creation. We now review the quasiprobability representations that are related to the results of this thesis.

[2]For example, there is a general disagreement on the quantum character of computational devices developed by the company D-wave [70]. Another example is the dispute about the cryptographic security of usual protocols of quantum key distribution [71].

2.2.1 Continuous representations

The phase space representation in terms of coherent states establishes a one-to-one correspondence between $|\alpha\rangle$ and a point $\alpha = \alpha_R + i\alpha_I$ on the complex plane, as explained in the preceeding chapter. In this fashion, distributions over the complex plane have a direct interpretation in terms of distributions on a classical configuration space, with α_R (α_I) corresponding to the position (momentum). An arbitrary operator in the coherent state representation correponds to a distribution over the phase space plane. In particular, density matrices arising from a classical process over a coherent state will be represented as probability distributions; the different interpretations of what a classical process means result in different probability distributions for these states. However, these diverse definitions share a common feature: it is impossible to represent every quantum state as a genuine probability distribution over the complex plane, as is evident from Theorem 1.

The characteristic function of an operator M is given by

$$\chi_M(\eta) = Tr[\rho e^{i\eta M}] \tag{2.1}$$

and gives all moments of this operator through the formula

$$\langle M^k \rangle = \frac{\partial^k}{\partial (i\eta)^k} \chi_M(\eta). \tag{2.2}$$

The natural choice in the phase-space picture is the displacement operator, giving a nice interpretation for the characteristic function as a generalized correlation function on the complex plane, by using (2.2) to obtain the moments of creation and annihilation operators. However, since these operators do not commute, the ordering convention has to be taken into account. The characteristic functions of the displacement operator in the antinormal, symmetric and normal ordering are respectivelly given by

$$\chi_A(\eta) = Tr\{\rho e^{-\eta^* a} e^{\eta a^\dagger}\}, \tag{2.3}$$

$$\chi_S(\eta) = Tr\{\rho e^{\eta a^\dagger - \eta^* a}\}, \tag{2.4}$$

$$\chi_N(\eta) = Tr\{\rho e^{\eta a^\dagger} e^{-\eta^* a}\}. \tag{2.5}$$

Since the characteristic function is a Fourier transform of the probability distribution in standard probability theory, the quasiprobability distributions are obtained performing an inverse Fourier transform of each characteristic function given above. From χ_N we obtain the Glauber-Sudarshan P distribution [26, 27]:

$$P(\alpha) = \frac{1}{\pi^2} \int_{-\infty}^{\infty} e^{\alpha\eta^* - \alpha^*\eta} \chi_N(\eta) d^2\eta \tag{2.6}$$

$$= \frac{1}{\pi^2} \int_{-\infty}^{\infty} e^{|\alpha|^2 + |\alpha'|^2} \langle -\alpha' | \rho | \alpha' \rangle e^{\alpha'^*\alpha - \alpha'\alpha^*} d^2\alpha'. \tag{2.7}$$

From χ_S we obtain the Wigner distribution [72]:

$$W(\alpha) = \frac{1}{\pi^2}\int_{-\infty}^{+\infty} e^{\alpha\eta^* - \alpha^*\eta}\chi_S(\eta)d^2\eta \tag{2.8}$$

$$= \frac{1}{\pi^2}\int_{-\infty}^{\infty} \langle\alpha - \alpha'|\rho|\alpha + \alpha'\rangle e^{\alpha'^*\alpha - \alpha'\alpha^*} d^2\alpha'. \tag{2.9}$$

And from χ_A we obtain the Husimi distribution [73]:

$$Q(\alpha) = \frac{1}{\pi^2}\int_{-\infty}^{+\infty} e^{\alpha\eta^* - \alpha^*\eta}\chi_A(\eta)d^2\eta = \frac{\langle\alpha|\rho|\alpha\rangle}{\pi}. \tag{2.10}$$

Each distribution has its proper peculiarities and advantages, with a large amount of uses in the literature, mainly in quantum optics. Let us briefly review each one.

Glauber-Sudarshan distribution

The P distribution in general can be more singular than the delta distribution or assign negative values to some regions of the phase-space, thus not qualifying as a genuine probability distribution. However, for some states the distribution does qualifies as a probability distribution and thus the state will behave classicaly in relation to the set of coherent states.

Observation 1 *An arbitrary state admits the following representation [74]:*

$$\rho = \int_{-\infty}^{+\infty} P(\alpha)|\alpha\rangle\langle\alpha|d^2\alpha, \tag{2.11}$$

where P is its Glauber-Sudarshan quasiprobability distribution.

Hence, whenever the P distribution qualifies as a legitimate probability distribution, the state is a statistical mixture of coherent states and in this sense is termed P-representable or classical. The interesting situations occur for states whose Glauber-Sudarshan distribution does not have this property. Then it is always possible to reveal this nonclassicality through interferometry experiments [74] and as will be shown in the next chapter, this nonclassicality can be used to create entanglement between the modes of radiation. The P quasiproability distribution is highly sensitive to nonclassicality in the optical domain, being in a certain sense the optimal detector of nonclassicality: if a state is not P-representable, than its Wigner distribution will be negative as well, but the converse is not true, i.e., there exists states with positive Wigner representation that are nonclassical for the P distribution. The price to be paid is the hardness of computing the Glauber-Sudarshan distribution, due to the highly nonsigular behaviour of nonclassical states.

Wigner distribution

The W distribution is perhaps the most used in practical applications of quasiprobabilities, with successfull uses in quantum tomography, quantum computation and semiclassical approximations. It is usual to write it in the coordinate representation:

$$W(q,p) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\langle q - x/2|\rho|q + x/2\rangle e^{ixp}dx. \tag{2.12}$$

For a pure state $\rho = |\psi\rangle\langle\psi|$, the wave function is $\psi(q) = \langle q|\psi\rangle$ and we have

$$\langle q - x/2|\rho|q + x/2\rangle = \psi^*(q - x/2)\psi(q + x/2), \tag{2.13}$$

so that the Wigner function is normalized to unity and real. A function $F^{(S)}(q,p)$ in symmetrical ordering of q and p obeys the relation

$$\langle F^{(S)}(q,p)\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} F^{(S)}(q,p)W(q,p)dqdp, \tag{2.14}$$

which has the structure of a classical ensemble average with q and p as random variables and $W(q,p)$ as the phase space density. The distinctive property of Wigner functions is the respect to the marginal distributions in phase space; for a pure state $\rho = |\psi\rangle\langle\psi|$, we have

$$\int_{-\infty}^{\infty} W(q,p)dp = |\psi(q)|^2, \tag{2.15}$$

$$\int_{-\infty}^{\infty} W(q,p)dq = |\tilde{\psi}(p)|^2. \tag{2.16}$$

Albeit its nice properties, the Wigner function displays negative values for many states and thus does not qualify as a genuine probability density function. This is not a disadvantage, though, since negativity in the Wigner function indicates some nonclassical feature of the optical field. Also, as we will see ahead, states with positive Wigner function are efficiently simulable in a classical computer, making negativity in the Wigner function a necessary condition for quantum computational speed-up. An important characterization in this sense is given by *Hudson's Theorem* [75]:

Theorem 2 *The Wigner function of a pure state $|\psi\rangle$ is positive iff $|\psi\rangle$ is a Gaussian state.*

For mixed states the situation is not so simple. Convex combinations of Gaussian states clearly have positive Wigner function, but there are mixed states with positive Wigner function which cannot be written as convex combinations of Gaussian states [76].

Husimi distribution

From the expression of the Husimi distribution

$$Q(\alpha) = \frac{\langle\alpha|\rho|\alpha\rangle}{\pi}, \tag{2.17}$$

we see directly that it is a positive distribution, since ρ is a positive semidefenite operator. It is also normalized to one and a smoothing of the Wigner function. It is indeed a probability distribution, however, it does not respects the marginal distributions in phase space. The Husimi is largely used in quantum optics and semiclassical approximations, since it is easy to calculate and it is a positive distribution. Its maximal value can be interpreted as a distance to the set of classical states and has many uses. One can also define the *Wehrl entropy* in the coordinate representation:

$$S_w(\rho) = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} Q(q,p)\ln Q(q,p)dqdp. \tag{2.18}$$

This entropy is a semiclassical approximation of the more general von Neumann entropy and measures the delocalization of the state in phase space [19].

The Cahill-Glauber formalism

It is possible to obtain quasiprobability distributions for any ordering of the annihilation and creation operators [77]. We define the filtered characteristic function,

$$\chi_\Omega(\beta, s) = \chi(\beta)\Omega_s(\beta), \tag{2.19}$$

where $\chi(\beta)$ is the usual characteristic function in normal ordering. Defining $\Omega_s(\beta) = e^{(s-1)|\beta|^2/2}$, one obtains the s-ordering of the creation and anihillation operators. The cases $s = 0, 1, -1$ correspond respectivelly to the W, P and Q distributions, while intermediate values give a continuous of novel quasiprobability distributions.

Extensions for generalized coherent states

The previous quasiprobability distributions were developed in terms of CCS, but the mathematical structure comes basically from Lie-group theory and thus the extensions to GCS are straightforward. Recalling the POVM resolution of identity

$$\int |\alpha_G\rangle\langle\alpha_G| d\mu(\alpha_G) = I, \tag{2.20}$$

where μ is the group-invariant measure, after some carefull steps [21, 19], we arrive at the generalized P distribution,

$$\rho = \int P(\alpha_G)|\alpha_G\rangle\langle\alpha_G| d\mu(\alpha_G), \tag{2.21}$$

and the generalized Q distribution

$$Q(\alpha_G) = \langle \alpha_G | \rho | \alpha_G \rangle. \tag{2.22}$$

As an example, let us see the case of $SU(2)$ symmetry. As we saw previously, the POVM resolution of identity is given by

$$\frac{2j+1}{4\pi} \int |z\rangle\langle z| d\Omega = I. \tag{2.23}$$

Hence, the Glauber-Sudarshan distribution is simply

$$\rho = \frac{2j+1}{4\pi} \int P(z)|z\rangle\langle z| d\Omega, \tag{2.24}$$

while the Husimi distribution is $Q(z) = \langle z|\rho|z\rangle$.

2.2.2 Discrete representations

Quasiprobability distributions for discrete systems are relativelly recent in comparison to their continuous counterparts. There is a great interest in discrete versions of the Wigner function, with each version adaptating some suitable feature of the continuous version. It is worthy mentioning the version given by Gross [78], which enabled important connections between the classicality notion associated to this version of the Wigner function and simulability in terms of the magic state model of quantum computation [79]. But, beyond the Wigner function, there are many recent developments of discrete quasiprobability distributions [5]. In this direction, we introduce a new quasiprobability representation in terms of MUB, with the main purpose of linking nonclassicality and complementary measurements. We will use this new representation in further sections to show how complementarity forbids the presence of phenomena beyond quantum theory.

Phase-space distributions

The discrete phase-space explained in the previous chapter enables us to translate the continuous quasiprobability distributions to the context of finite geometry. The treatment given here follows [32]. The displacement operator in finite dimension d, as we saw, is given by

$$T(a_1, a_2) = \omega^{-a_1 a_2/2} Z^{a_1} X^{a_2}, \quad (a_1, a_2) \in Z_d \times Z_d. \tag{2.25}$$

The characteristic or Weyl function is defined as usual taking the mean value of the displacement operator:

$$\xi(a_1, a_2) = Tr[\rho T(a_1, a_2)]. \tag{2.26}$$

Introducing the parity operator at the origin $P(0,0) = F^2$, with F the finite Fourier transform (1.22), we have that the Wigner function is given by

$$W(a_1, a_2) = Tr[\rho P(a_1, a_2)], \tag{2.27}$$

where $P(a_1, a_2) = T(a_1, a_2)P(0,0)T^{\dagger}(a_1, a_2)$ is the parity-displaced operator[3] at the point (a_1, a_2). It is also possible to show that the characteristic and Wigner functions are related throug a double Fourier transform:

$$\xi(a_1, a_2) = \frac{1}{d} \sum_{a_1', a_2'=0}^{d-1} W(a_1', a_2') \omega^{a_1 a_2' - a_2 a_1'}. \tag{2.28}$$

The Wigner function respects the marginal property:

$$\frac{1}{d} \sum_{a_2=0}^{d-1} W(a_1, a_2) = \langle a_1 | \rho | a_1 \rangle, \tag{2.29}$$

$$\frac{1}{d} \sum_{a_1=0}^{d-1} W(a_1, a_2) = \langle a_2 | \rho | a_2 \rangle. \tag{2.30}$$

The construction can be generalized for s-ordering [80], where as usual $s = 1, 0, -1$ corresponds respectivelly to the Husimi, Wigner and Glauber distributions. It is shown also that the continuous limit is precisselly the continuous Cahill-Glauber formalism.

2.2.3 Quasiprobability distribution for MUB

Before presenting our approach, we stress that there are other approaches for quasiprobability distributions in terms of MUB [81, 82]. Our approach, however, seems to be a more explicit representation and has a nice geometrical picture in terms of barycentric coordinates. Also, it is easy to manipulate in order to construct examples of preparations and measurements for some determinate problems. The main idea is to represent positively the states in the convex hull of some fixed set of MUB, so that we have a genuine probability distribution in this set and hence we can label the corresponding

[3] Similar relations are valid for the continuous Wigner function as well, although we did not show this in previous sections.

states as classical. This polytope appears in many different situations in the literature [43, 47, 48, 83, 84, 85], which is one big motivation for this construction. Also, any state outside this polytope will display some negative weight in the representation, thus being nonclassical in this sense. Moreover, the representation is unique due to the use of barycentric coordinates footnoteThe barycentric coordinates of a point $\mathbf{x}$ in a convex set with fixed points $\mathbf{x}_i$, $i = 0, 1, \ldots, n$, are the values μ_i such that $\mathbf{x} = \mu_0\mathbf{x}_0 + \mu_1\mathbf{x}_1 + \ldots + \mu_n\mathbf{x}_n$ and $\mu_0 + \mu_1 + \ldots + \mu_n = 1$. and a tricky avoidance of Caratheodory's Theorem[4]. In the next section, we will apply the representation to study the clash between complementarity and superquantum configurations.

Construction of the representation for a qubit

Let us start with the simplest situation of a qubit, the central tool in the quantum theory of information. In this special case, the construction can be elegantly stated in terms of the l_1-norm of the three-dimensional Bloch vector. Let us start with some important definitions and properties.

Given a vector $\mathbf{v} = (v_0, v_1, v_2, \ldots)$ in some vector space $\mathcal{V}$, its l_p-norm is given by

$$||\mathbf{v}||_p = \left(\sum_i |v_i|^p\right)^{1/p} \tag{2.31}$$

Each value of p corresponds to a different unit-ball, as depicted in Fig. 2.1. We will restrict the discussion to values $1 \leq p \leq \infty$, since in these cases the unit-balls are convex bodies. In three dimensions, $\mathbf{v} = (v_0, v_1, v_2)$, the set of points at unit distance or less from the origin ranges from a solid octahedron - points that satisfy $||\mathbf{v}||_1 = |v_0| + |v_1| + |v_2| \leq 1$ - to a ball - points satisfying $||\mathbf{v}||_2 = \sqrt{|v_0|^2 + |v_1|^2 + |v_2|^2} \leq 1$ - and finally to a solid cube - points that satisfy $||\mathbf{v}||_\infty = \lim_{p\to\infty} ||\mathbf{v}||_p = \max\{|v_0|, |v_1|, |v_2|\} \leq 1$.

It is well known that an arbitrary state of a qubit admits a Bloch-vector representation:

$$\rho = \frac{1}{2}(I + \mathbf{r} \cdot \sigma) \tag{2.32}$$

which can be rewritten in terms of the l_2-norm as

$$\rho = \frac{1}{2}(I + ||\mathbf{r}||_2(\mathbf{n} \cdot \sigma)) \tag{2.33}$$

[4]This theorem states that if X is a subset of R^n, then any point in the convex hull of X can be expressed as a convex combination of at most $n + 1$ points in X.

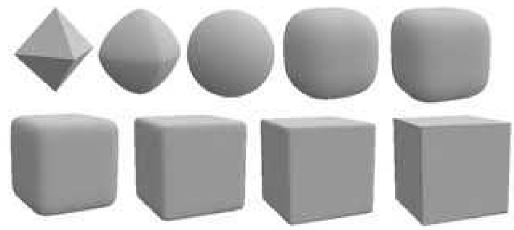

Figure 2.1: Three-dimensional unit-balls associated to l_p-norms for each value of p. For $p = 1$, the unit-ball describes an octahedron, which coincides with the complementarity polytope defined in [43]. The following figure is a deformed octahedron, associated to $p = 3/2$. The next body is a solid sphere, corresponding to $p = 2$. The process goes on and in the limit of $p = \infty$ culminates in a solid cube.

where $\mathbf{n} = \mathbf{r}/||\mathbf{r}||_2$ is a directional unit vector in the three-dimensional space. It is easy to see that for $||\mathbf{r}||_2 \leq 1$, i.e., the unit-ball for the l_2-norm, the states are positivelly represented, while $||\mathbf{r}||_2 > 1$ the states display negative values. What could be said about other norms?

We will focus in the l_1-norm of the Bloch vector, which is simply $||\mathbf{v}||_1 = \sum_i |v_i| = |v_0| + |v_1| + |v_2|$. The reasons for this choice will become evident in the next section. The l_1-norm induces a distance between vectors known as the *Manhattan distance* or *taxicab distance*[5]. Rewriting (2.32) in terms of the l_1-norm, we get

$$\rho = \frac{1}{2}(I + \mathbf{r} \cdot \sigma) = \frac{1}{2}(I + ||\mathbf{r}||_1 \mathbf{r}' \cdot \sigma) \tag{2.34}$$

where $\mathbf{r}' = (\mathbf{r}/||\mathbf{r}||_1) \equiv (x', y', z')$. Since $||\mathbf{r}'||_1 = |x'| + |y'| + |z'| = 1$, we have

$$\begin{aligned}
\rho &= \frac{1}{2}((|x'| + |y'| + |z'|)I + ||\mathbf{r}||_1 \mathbf{r}' \cdot \sigma) && (2.35)\\
&= \frac{1}{2}(|x'|I + ||\mathbf{r}||_1 x'\sigma_x) + \frac{1}{2}(|y'|I + ||\mathbf{r}||_1 y'\sigma_y) + \frac{1}{2}(|z'|I + ||\mathbf{r}||_1 z'\sigma_z) && (2.36)\\
&= \frac{1}{2}(|x'|(P_{x+} + P_{x-}) + ||\mathbf{r}||_1 x'(P_{x+} - P_{x-})) && (2.37)\\
&+ \frac{1}{2}(|y'|(P_{y+} + P_{y-}) + ||\mathbf{r}||_1 y'(P_{y+} - P_{y-})) && (2.38)\\
&+ \frac{1}{2}(|y'|(P_{z+} + P_{z-}) + ||\mathbf{r}||_1 z'(P_{z+} - P_{z-})). && (2.39)
\end{aligned}$$

where $P_{i\pm}$ are the projectors on the various elements of the MUB set. Here, instead of making the usual identification $P_{i\pm} \equiv |i\pm\rangle\langle i\pm|$, we let open the interpretation

[5] The name comes from the observavtion that in Manhattan, the streets form a square grid and a taxicab driver will perform displacements either horizontally or vertically, but not diagonally [19].

of these projectors as preparations, independently on the Hilbert space formalism of quantum mechanics. Following Peres [1], we are representing an arbitrary preparation in terms of the maximal tests encoded on the projectors. We arrive at the following representation:

$$\begin{aligned}\rho &= \frac{|x'|+||\mathbf{r}||_1 x'}{2}P_{x+}+\frac{|x'|-||\mathbf{r}||_1 x'}{2}P_{x-}+\frac{|y'|+||\mathbf{r}||_1 y'}{2}P_{y+}\\ &+ \frac{|y'|-||\mathbf{r}||_1 y'}{2}P_{y-}+\frac{|z'|+||\mathbf{r}||_1 z'}{2}P_{z+}+\frac{|z'|-||\mathbf{r}||_1 z'}{2}P_{z-}\\ &= w(x+)P_{x+}+w(x-)P_{x-}+w(y+)P_{y+}+w(y-)P_{y-}+w(z+)P_{z+}+w(z-)P_{z-},\end{aligned}$$

which we write as

$$\rho = \sum_{\substack{i=x,y,z\\ \nu=+,-}} w(i\nu)P_{i\nu}, \tag{2.40}$$

where we labeled $w(i\pm) = (|i'| \pm ||\mathbf{r}||_1 i')/2$, with $i = x, y, z$. The functions $w(i\nu)$ satisfy all requirements for a (discrete) probability distribution over the projectors on MUB, except that they can become negative for some states. It is easy to see that this happens whenever $||\mathbf{r}||_1 > 1$ while for $||\mathbf{r}||_1 \leq 1$, we have true probability distributions, i.e., the functions $w(i\mu)$ are all positive. In the latter case we say that the state is classical. Notice the total analogy between the quasiprobability representation (2.40) and the Glauber-Sudarshan representation (2.11): in both representations, classical states are those represented as convex combinations of the pure classical states, while nonclassical states are those that display negative values for the distribution.

The relation to Definition 3 is done if we identify $\lambda \equiv i\nu$, i.e., the ontic parameter is given by the complementary directions $x\pm$, $y\pm$, $z\pm$; this resembles very much the construction in [83]. Also, the functions in Definition 3 are given by $\mu_\rho(\lambda \equiv i\nu) = w(i\nu)$ and[6] $\xi_E(\lambda) = Tr(EP_{i\nu})$. Let us see the geometry associated to the set of classical states and then proceed to justify further this terminology.

Geometric interpretation

As implied by the discussion on l_p-norms, states with positive quasiprobability representation (2.40) - i.e., classical in the sense of MUBs - are contained in an octahedron inscribed in the Bloch ball, as is depicted in Fig. 2.2. The pure classical states of this distribution are the elements of the MUB set and sit at the vertices of the octahedron. The mixed states are at the faces and interior of the polyhedron and it is straightforward that this convex body is exactly the convex hull of the elements of MUB, or, in

[6]

other words, the complementarity polytope [43]. This geometrical structure appears in very important scenarios of quantum information theory. The Gottesmann-Knill theorem and related quantum computation models based on discrete versions of the Wigner function imply that classical states here are efficiently simulated by a classical computer [47, 48, 79]. From the foundational side, the classical states are fully described by an ontological model [83, 84, 85], i.e., are classically represented. Thus, the terminology is well justified.

In order to get a geometrical picture of the quasiprobability distribution, let us consider the special case where the l_1-normalized coordinates x',y', z' are positive. Then we can rewrite the representation of the state as

$$\begin{aligned} \rho &= \frac{1+||\mathbf{r}||_1}{2}(x'P_{x+} + y'P_{y+} + z'P_{z+}) + \frac{1-||\mathbf{r}||_1}{2}(x'P_{x-} + y'P_{y-} + z'P_{z-}) \\ &= \lambda\rho_+ + (1-\lambda)\rho_-, \end{aligned} \tag{2.41}$$

where $\lambda = \frac{1+||\mathbf{r}||_1}{2}$ and $\rho_\pm$ are states whose Bloch vectors lie in the antipodal faces depicted in Fig. 2.2.

In this picture the coordinates x',y', z' are barycentric coordinates on the faces that contain $\rho_\pm$. Since barycentric coordinates are unique, all states in the interior of the octahedron are *unambiguously* described as mixtures of antipodal states sitting in the faces of the octahedron. The small price we pay for this uniqueness is a certain redundancy in the description, since we are not using the full power of Caratheodory's Theorem. The theorem says that we *could* always represent the interior points as mixtures of at most $3+1 = 4$ extremal states, but it does not forces us to do so. Indeed, if we choosed this minimal representation, we would have always to force a convention on the fourth extremal point and there would be an ambiguity, which would bring an extra pointless problem. Here, classical states are uniquelly represented as convex combinations of all six extremal states, while nonclassical states demand negatives values for the mixing parameter λ in order to be represented. Since in higher dimensions there is not a direct relation with l_p-norms of the Bloch vector, we will use the idea of performing mixtures or quasi-mixtures of states in the faces of the complementarity polytope in order to construct quasiprobability representations in arbitrary (prime power) dimensions.

Examples

The elements of the MUB are pure states with $||\mathbf{r}||_1 = 1$ and are the vertices of the octahedron; the state $|z+\rangle = |0\rangle$ has the obvious distribution $w(z+) = 1$, $w(x\pm) =$

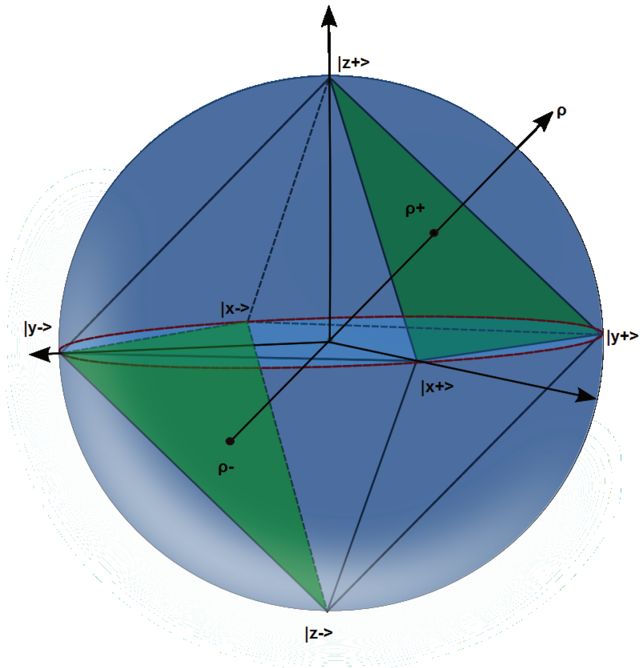

Figure 2.2: The set of classical states is given by the $||\mathbf{r}||_1$ unit-ball, an octahedron that has as extreme points the elements of the MUB set. The set of configurations allowed by quantum mechanics is given by the $||\mathbf{r}||_2$ unit-ball, the well-known Bloch-ball. The configuration ρ, as described in (2.41), is a quasi-mixture of antipodal states $\rho_{\pm}$. The state ρ_+ is in the face defined by $\{|x+\rangle, |y+\rangle, |z+\rangle\}$, while ρ_- is in the face defined by $\{|x-\rangle, |y-\rangle, |z-\rangle\}$. Both states have barycentric coordinates (x', y', z') in relation to the extremal points of their respective faces.

$w(y\pm) = w(z-) = 0$, for example. The state $\rho_+ = \frac{1}{2}[I + (\sigma_x + \sigma_y + \sigma_z)/3]$ sits in the center of the face formed by the states $|x+\rangle$, $|y+\rangle$ and $|z+\rangle$, thus having barycentric coordinates $x' = y' = z' = 1/3$, $||\mathbf{r}||_1 = 1$ and hence the distribution is $w(x+) = w(y+) = w(z+) = 1/3$, $w(x-) = w(y-) = w(z-) = 0$. As an example of a nonclassical state, we consider the magical state $\rho_T = \frac{1}{2}[I+(\sigma_x+\sigma_y+\sigma_z)/\sqrt{3}]$, for which $||\mathbf{r}||_1 = \sqrt{3}$, thus implying $w(x\pm) = w(y\pm) = w(z\pm) = (1 \pm \sqrt{3})/6$, displaying negative values for the distribution, since $(1 - \sqrt{3})/6 < 0$. Another way of seeing this case is noticing that $\rho_T = (1 - \lambda)\rho_+ + \lambda\rho_-$, with $\lambda(1 - \sqrt{3})/2 < 0$ and $\rho_{\pm} = \frac{1}{2}[I \pm (\sigma_x + \sigma_y + \sigma_z)/3]$ are the states in the antipodal faces, thus requiring negative values of the mixing parameter λ in order to represent the state.

Higher dimensions

For dimensions $d > 2$ the geometry is far more complicated and there are many different Bloch vector parametrization of density matrices [19, 86] (see also references in [41]). Here it is better to form mixtures or quasi-mixtures of states in disjoint faces of the MUB polytope. Let us see the case of a qutrit in detail; the other cases will be straightfoward extensions. There are 4 MUB given by $\mathcal{B}_i = \{|0^{(i)}\rangle, |1^{(i)}\rangle, |2^{(i)}\rangle\}$, with $i = 1, 2, 3, 4$ and the elements are explicitly written in (1.61). The disjoint faces are composed of four elements of each MUB and we can form three of them "per turn", i.e., per hyperoctant; for example, we form the faces

$$\begin{aligned} F_0 &= \{|0^{(1)}\rangle, |0^{(2)}\rangle, |0^{(3)}\rangle, |0^{(4)}\rangle\}, \\ F_1 &= \{|1^{(1)}\rangle, |1^{(2)}\rangle, |1^{(3)}\rangle, |1^{(4)}\rangle\}, \\ F_2 &= \{|2^{(1)}\rangle, |2^{(2)}\rangle, |2^{(3)}\rangle, |2^{(4)}\rangle\} \end{aligned} \tag{2.42}$$

and then assign the states living in each face

$$\rho_0 = \sum_{i=1}^{4} p_i |0^{(i)}\rangle\langle 0^{(i)}|, \tag{2.43}$$

$$\rho_1 = \sum_{i=1}^{4} p_i |1^{(i)}\rangle\langle 1^{(i)}|, \tag{2.44}$$

$$\rho_2 = \sum_{i=1}^{4} p_i |2^{(i)}\rangle\langle 2^{(i)}|. \tag{2.45}$$

Notice that the barycentric coordinates p_i are the same for the three states. Now, we form states by mixtures or quasi-mixtures of the face states above:

$$\rho = \lambda_0\rho_0 + \lambda_1\rho_1 + \lambda_2\rho_2, \tag{2.46}$$

where $\lambda_0+\lambda_1+\lambda_2 = 1$ and we let the values λ_i assume any real value. A nice implication is that we can rewrite this expression as

$$\rho = \sum_{i=1}^{4} p_i(\lambda_0|0^{(i)}\rangle\langle 0^{(i)}| + \lambda_1|1^{(i)}\rangle\langle 1^{(i)}| + \lambda_2|2^{(i)}\rangle\langle 2^{(i)}|), \tag{2.47}$$

as if we formed the state through barycentric coordinates of the orthogonal simplices of each basis. As an example, let us consider the barycentric coordinates $p_1 = p_2 = p_3 = p_4 = 1/4$ and let us form a state using (2.46) and simplifying the parametrization to $\lambda_0 = (1 - 2\lambda')$, $\lambda_1 = \lambda_2 = \lambda'$. In matricial representation, we have

$$\rho = \frac{1-2\lambda'}{4}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} + \frac{\lambda'}{4}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{pmatrix}. \tag{2.48}$$

It is easy to find numerically that $\lambda' = 1$ corresponds to the pure state $(|2\rangle - |1\rangle)/(\sqrt{2})$ and the quasiprobability representation is then given by:

$$\rho = \frac{1}{4}\left(\sum_{i=1}^{4} |1^{(i)}\rangle\langle 1^{(i)}| + |2^{(i)}\rangle\langle 2^{(i)}| - |0^{(i)}\rangle\langle 0^{(i)}|\right). \qquad (2.49)$$

States in diverse hyperoctants are obtained simply by permutation of the elements in each face (2.42). The extension to higher dimensions is straightforward: we separate the elements of the MUB set in d disjoint faces containing $d+1$ elements. We then pick states in each face with the same barycentric coordinates. Finally, we perform mixtures or quasimixtures of these face states and obtain the states we want.

2.3 Complementarity versus superquantum configurations

The quasiprobability representation just constructed assigns positive weights to states inside the complementarity polytope, while those outside this polytope necessarilly display some negativity. Thus, to represent all states we have to relax the axiom of probability that demands positive probability weights. However, nothing is forcing us to impose the rules of quantum theory; in our representation quantum states outside the complementarity polytope share the same status as non-quantum ones, in the sense of requiring negative values in the quasiprobability distribution. Considering that Born's rule corresponds with good precision to the probabilities measured in laboratory, it is evident that by not imposing the axioms of quantum physics, i.e., allowing any weight in the representation, we will eventually step in actual negative values of probability for measurements. Although this is surelly a strange route to take, it is not totally new in quantum mechanics [89]. Contemporary measurement theory actually uses negative probabilities - and even complex probabilities - in the formalism of weak measurements [87, 88], which is a topic of increasing interest in the literature. Also, one can use negative probabilities to represent superquantum nonlocality [90]. We will follow these ideas in order to define superquantum configurations, i.e., preparations beyond quantum formalism which can be used to break the limits imposed by the theory. Focusing in the case of a qubit, we will show that in a certain sense one can regard some of these configurations as valid, if a restriction to complementary measurements and a simple contextual model are accepted. Equipped with the relations developed by Luis [50], we will show that every superquantum configuration violates the complementarity principle, even assuming negative probabilities as a valid description. Since states of many qubits can be generated through activation protocols over individual qubits, the results will be valid for $d = 2^n$ as well, which is the usual situation in quantum information theory. Hence, it is proved that future research will have to abandon either the marvels of superquantum configurations [14], or the complementarity principle.

2.3.1 Tsirelson's bound

For a qubit, the quasiprobability representation of the previous section displays negative weights for preparations outside the octahedron of classical states. Without resorting to the postulates of quantum mechanics, it is not possible to discriminate between quantum preparations or non-quantum ones, i.e., preparations outside the Bloch sphere. Let us assume then that all these preparations are valid, without imposing the requirement of positive semidefiniteness on the operators representing the states. Also, we will assume that we have any quantum operation at our disposal. Thus, a valid preparation would be the following quasi-mixture of complementary projectors

$$\rho = (1+\epsilon)P_{x+} - \epsilon P_{z+}, \tag{2.50}$$

with ϵ being any real number. Now, we perform a CNOT operation[7] over the state $\rho \otimes |z+\rangle\langle z+|$, obtaining

$$\rho_f = (1+\epsilon)P_{\phi+} - \epsilon P_{z+} \otimes P_{z+} \tag{2.51}$$

where $P_{\phi\pm} = |\phi^\pm\rangle\langle\phi^\pm|$ and $|\phi^\pm\rangle = (1/\sqrt{2})(|00\rangle \pm |11\rangle)$. As we saw previously, there is a configuration of local measurements such that the Bell-operator (1.85) obeys $|\langle B(\phi+)\rangle| = 2\sqrt{2}$, reaching Tsirelson's bound. Let us estimate the bound attained for ρ_f:

$$|\langle B(\rho_f)\rangle| = |\langle (1+\epsilon)B(\phi+) - \epsilon B(|z+, z+\rangle\langle z+, z+|)\rangle| \tag{2.52}$$

We can choose easilly local observables such that $\langle B(|z+, z+\rangle\langle z+, z+|)\rangle = 0$, while $\langle B(\phi+)\rangle$ is maximal: it is just a matter of taking the local observables on the x, y plane, since $\langle z+|\sigma_x|z+\rangle = \langle z+|\sigma_y|z+\rangle = 0$. Thus we get $|\langle B(\rho_f)\rangle| = (1+\epsilon)|\langle B(\phi+)\rangle| = (1+\epsilon)2\sqrt{2}$, an *arbitrary violation* of the Tsirelson's bound depending directly on the parameter ϵ.

We saw that the maximal violation for an arbitrary nonlocal box is bounded by 4, the algebraic maximum of $|\langle B(\rho_f)\rangle|$. However, this is true if one is dealing with

[7] Defined in (3.12). See the discussion in Section 3.3 for a better understanding.

non-negative values of probability. We thus have a correspondence with nonlocal boxes predictions if we impose a bound on the quasi-mixture parameter of $\epsilon = \sqrt{2}-1$; higher values originate configurations other than nonlocal boxes, which is a subject to be investigated elsewhere. This example is very general, since any configuration outside the Bloch ball of quantum states can be locally rotated to (2.50) and then used to create states with superquantum nonlocality. Due to this we will give the label *superquantum configuration* to any preparation outside the set of quantum states.

2.3.2 Distinguishability and no-cloning

Superquantum configurations respect the linearity of quantum mechanics and thus it is expected that some kind of no-cloning theorem still applies. We show now that this is true through an extended version of the theorem:

Theorem 3 *Two states ρ and ρ' are clonable by a same unitary U only if $Tr(\rho\rho') = 0$ or $Tr(\rho\rho') = 1$.*

Proof: If ρ and ρ' are clonable by a unitary U, then we have

$$U(\rho \otimes |e_0\rangle\langle e_0|)U^\dagger = \rho \otimes \rho \tag{2.53}$$

$$U(\rho' \otimes |e_0\rangle\langle e_0|)U^\dagger = \rho' \otimes \rho' \tag{2.54}$$

We then have

$$Tr[(\rho \otimes \rho)(\rho' \otimes \rho')] = Tr[U(\rho \otimes |e_0\rangle\langle e_0|)U^\dagger U(\rho' \otimes |e_0\rangle\langle e_0|)U^\dagger] = Tr(\rho\rho') \tag{2.55}$$

where we used the cliclicity of trace in the last step. Since $Tr(A \otimes B) = Tr(A)Tr(B)$, the first term is equal to $[Tr(\rho\rho')]^2$. Thus we have

$$[Tr(\rho\rho')]^2 = Tr(\rho\rho') \tag{2.56}$$

as a condition to existence of a unitary U that clones ρ and ρ'. This is equivalent to $Tr(\rho\rho') = 0$ or $Tr(\rho\rho') = 1$, QED.

The equations $Tr(\rho\rho') = 0$ or $Tr(\rho\rho') = 1$ are those of parallel hyperplanes. When restricted to quantum mechanics, it is only possible to satisfy these relations for orthogonal pure states. However, when we allow configurations beyond quantum mechanics, it indicates a possibility of cloning mixed states as well, without resorting to ancillary extensions. This would be a huge improvement, since augmentation of a system can be very challenging in practice. Also, $Tr(\rho\rho') = 0$ means that ρ and ρ' are ortoghonal in the Hilbert-Schmidt inner product. For pure states it is easy to show that this implies total distinguishability between the states: performing the projective measurement on one of the states, the result 0 ou 1 will discriminate one from the other. For superquantum configurations, an analogous discrimination can be established by the use of generalized measurements.

Let us see how this applies in the qubit case. It is simple to see that in terms of the Bloch vector, we have

$$Tr(\rho\rho') = \frac{1}{2}(1 + \mathbf{r} \cdot \mathbf{r}') \tag{2.57}$$

It is possible to clone two arbitrary configurations with an unitary U only if

$$\mathbf{r} \cdot \mathbf{r}' = \pm 1 \tag{2.58}$$

These are the equations of two affine hyperplanes that cross the interior of the Bloch ball, whenever at least one of the states ρ, ρ' is a superquantum configuration.

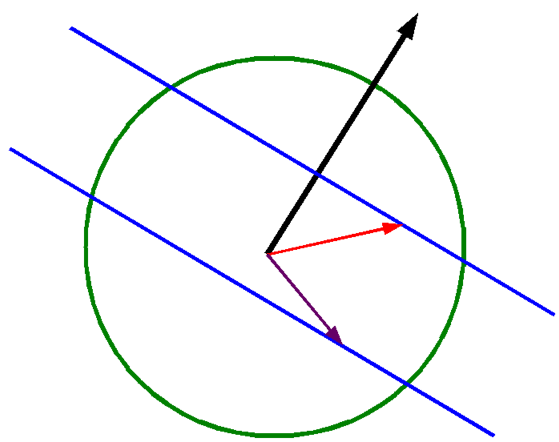

Figure 2.3: A superquantum configuration (in black) defines two planes (in blue) crossing the Bloch sphere (in green). These planes are formed by the states that can in principle be cloned together with the superquantum state by the same unitary. In the Bloch representation, if $\mathbf{r}$ is the Bloch vector of the superquantum state (in black), then a state respecting $\mathbf{r} \cdot \mathbf{r}' = 1$ (in red) or a state respecting $\mathbf{r} \cdot \mathbf{r}' = -1$ (in violet) have this property.

2.3.3 Restrictions by probability theory

We can restrict the set of allowed states or preparations if we further impose that the probability given by a projective measurement in a MUB be trully a probability, i.e, nonnegative, smaller or equal to unity and suming up to one. Thus, we can rule out, for example, a matrix given by

$$\rho = \frac{1}{2}(I + (1+\delta)\sigma_z) \tag{2.59}$$

for all $\delta > 0$. For this matrix, $Tr(|0\rangle\langle 0|\rho) = 1+(\delta/2)$ and $Tr(|1\rangle\langle 1|\rho) = -(\delta/2)$, which clearly violates the basic laws of probability. We can then prove the following:

Observation 2 *The set of states allowed by probability theory is bounded by the* $||\mathbf{r}||_\infty$ *unit-ball.*

Proof: The l_∞-norm of the Bloch vector is $||\mathbf{r}||_\infty = \max\{|r_x|, |r_y|, |r_z|\}$. Let us first consider that the Bloch vector has positive values r_i, $i = x, y, x$; then $|r_i| = r_i$ and the vectors inside the $||\mathbf{r}||_\infty$ unit-ball are those for which $||\mathbf{r}||_\infty = \max\{r_x, r_y, r_z\} \leq 1$. Thus, in the situation of positive values of the Bloch vector, an arbitrary preparation outside the $||\mathbf{r}||_\infty$ unit-ball can be parameterized through

$$\rho = \frac{1}{2}(I + (1+\delta_x)\sigma_x + (1+\delta_y)\sigma_y + (1+\delta_z)\sigma_z) \tag{2.60}$$

for $\delta_i > 0$, since in this case we have $||\mathbf{r}||_\infty = \max\{1+\delta_x, 1+\delta_y, 1+\delta_z\} = \max\{1,1,1\} + \max\{\delta_x, \delta_y, \delta_z\} = 1 + \max\{\delta_x, \delta_y, \delta_z\} > 1$. A measurement of any σ_i in the state (2.60), for $i = x, y, z$ yields outcome $+1$ with probability $1 + (\delta_i/2)$ and -1 with probability $-(\delta_i/2)$. Hence, for any $\delta_i > 0$ there is a violation of normalization or non-negativity rules of probability theory, implying that the only way to have allowed configurations is that $\delta_i \leq 0$. Now, the situation is symmetrical under reflections of the Bloch-ball, thus this example exhausts all examples of states outside the $||\mathbf{r}||_\infty$ unit-ball, which thus violate probability theory, QED.

This dual structure[8] appears in the related reference [84], where a hidden variable theory enabling an efficient simulation of the states in the octahedron of classical states is given, using the vertices of the cube. A more foundational approach is given by [83], where the cube construction is implicit. We stress that besides the significant reduction on the allowed preparations, we see that standard probability theory does

[8]The $||\mathbf{r}||_\infty$ unit-ball is the dual polytope of the $||\mathbf{r}||_1$ unit-ball [19].

not eliminate completely the presence of superquantum configurations. This can be seen as a consequence of the two paradigms of quantum theory, one for describing the temporal evolution of a state by reversible tranformations and the other to describe measurements, in which the act of observing the system irreversibly alters the state.

One could reason, for example, that the superquantum states outside the Bloch ball but inside the dual cube - i.e., respecting $||\mathbf{r}||_2 > 1$ but $||\mathbf{r}||_\infty < 1$ - could be rotated to (2.50), through an unitary transformation. With this state in hand, we could violate Tsirelson's bound and perform tasks beyond quantum theory. From the measurement viewpoint, however, one realizes that a projective measurement in the direction of this superquantum Bloch vector already displays a negative value, since for this state one has $||\mathbf{r}||_2 > 1$. Thus, reasoning in terms of what is observed implies that quantum mechanics would be restored by measuring on all directions and observing which preparations respect standard probability theory. This, however, has some hidden assumptions that are not firmly grounded. The first is to consider that we could observe such violations of probability theory, in case they occured. But how to interpret a negative probability? For the frequentist interpreation, it would be a nonsense requirement, while for other interpretations such probabilities should be discarded as part of errors and fluctuations. Following [91] in a different perspective, perhaps such events really occur, but our interpretation in terms of probabilities is bounding us to give an answer to what is observed in a biased way. The situation would be like a blind person claiming that the sun does not exist on the basis that he only sees the black color. In order to correctly rule out phenomena beyond quantum theory, we must avoid taking conclusions based solely on the probabilities of outcomes, since in quantum regime the non-observability of a phenomenon does not imply its non-existence or impossibility of use: as already said, one could could rotate a superquantum configuration to (2.50) through an unitary transformation (deterministic operation) and use this state to perform superquantum tasks, even though being unable to interpret it correctly. A second argument against such kind of approaches based on observability is given in what follows, where we consider a contextual model of measurements which would leave open the existence of superquantum configurations.

2.3.4 Restrictions by the complementarity principle

The complementarity of measurements on conjugate variables is a well-observed phenomena in experiments [39]. However, there is in fact at least one experiment claiming that the complementarity principle can be violated, the very much controversial Afshar's experiment[9] [93]; while its conclusions are considered wrong, we consider here the consequences of a hypothetical violation of the complementarity principle in discrete systems. This is motivated also by claims of observation of negative probabilities by using weak measurements [88].

We will restrict the measurements to those on MUB, given that the collection of such measurements is Informationally Complete (IC). This has some conceptual advantages as well. When measuring on MUB, we are collecting information between complementary aspects of a state. Measurements on non-MUB directions leave open other interpretations, since the bias towards one of the directions could have different explanations. In this situation, the experimental arrangements are not fully excludent. One could of course rotate the complementarity polytope to these other directions and claim to observe the supremacy of quantum mechanics, i.e., proceed to not observe negative probabilities. However, besides the connundrum described in the end of the previous section, we would be implicitly and needlessly invoking the quantum postulate on the dynamical evolution of a state and then weakening our argumentation. We are trying to assume nothing more than the data collected by IC complementary measurements.

Moreover, we can envisage a model of measurement which would correspond to quantum mechanics in the Bloch sphere, but that allows superquantum states in the probability dual cube explained previously. The idea is simple: let us imagine that a measurement $\sigma \cdot \hat{\mathbf{n}}$ in a direction $\hat{\mathbf{n}}$ rotates the configuration cube so that it coincides with the cube associated to the complementary measurements associated to the direction $\hat{\mathbf{n}}$. This maybe sounds strange, since it is as if the observation influences somehow the preparation prior to the measurement. However, this is a common feature in quantum measurements if one remembers the acts of pre-selection and post-selection [124, 6], which are well-established models of measurement. The model is clearly preparation and measurement contextual, but this is not exactly a problem, since quantum mechanics alone is contextual and the situation resembles the 3-box Paradox described in [94]. Hence, measuring in arbitrary directions could assume this possible contextual model, allowing superquantum states that are coincidental with quantum theory upon observation, but that could in principle activate superquantum nonlocality as described previously. Thus, restricting the measurements to MUB directions is a better option, since we have to assume less premisses as true.

[9]The transactional interpretation of quantum mechanics [92] claims that there is not a contradiction with quantum mechanics in this experiment; the contradiction would come from the Copenhagen interpretation, which would then be wrong.

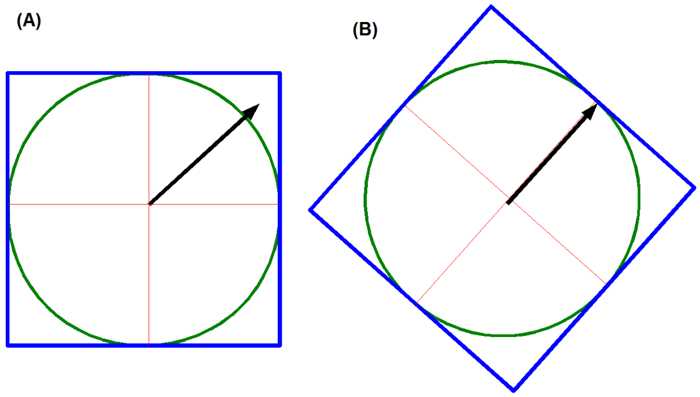

Figure 2.4: In (A), a superquantum configuration (in black) allowed by probability theory: it is a preparation outside the Bloch ball (in green) but inside the probability cube (in blue). The structure is defined by the MUB directions (in red). In (B) we represent a possible model of measurements that coincides with quantum mechanics: if one measures in the direction of the superquantum state (black), a new configuration cube (blue) associated to the new MUB set (red) is established and the measurement coincides with the predictions of quantum mechanics, since the tip of the superquantum states "collapses" to the pure state in the Bloch ball (green). No violation of the quantum probability rules would be observed in this model, but superquantum states would still be available. In part (A) the superquantum state could be rotated to (2.50) and then used to activate superquantum nonlocality, only by the use of unitaries, which are deterministic operations.

We show now that superquantum states violate the complementarity of measurements in MUB, even if we do assume the presence of negative probabilities. Let us take an extreme example to illustrate the idea, the superquantum state given by

$$\rho = \frac{1}{2}(I + \sigma_x + \sigma_y + \sigma_z) \tag{2.61}$$

It is an straightforward calculation that $Tr(|i+\rangle\langle i+|\rho) = 1$ and $Tr(|i-\rangle\langle i-|\rho) = 0$ where $i = x, y, z$; these probabilities are observed *independently* on which MUB we choose to measure. This is a clear violation of the complementarity principle. Another way of seeing this is computing entropic uncertainty relations on this matrix for two MUB, or even the whole set of MUB. The result is $H_{B_1} + H_{B_2} = 0$, which is an enormous violation of the relation for MUB (1.46). Let us see now how these ideas can be seen in the general case.

As explained previously, the quantitative complementarity relations developed by Luis have clear advantages over uncertainty relations. Also, there is nothing forbidding us of using negative numbers for the probabilities. Let us see how this applies for the simple situation of a qubit. In this case, relation (1.53) for measurements in the three MUB gives

$$C_x^2 + C_y^2 + C_z^2 \leq 2 \tag{2.62}$$

The probabilities of projective measurements in MUB is given by

$$p(i\pm) = \frac{1}{2}(1 \pm r_i) \tag{2.63}$$

for $i = x, y, z$ and thus the complementarity relation demands that $r_x^2 + r_y^2 + r_z^2 \leq 1$, i.e., $||\mathbf{r}||_2 \leq 1$ which means that the allowed configurations *must be inside the Bloch ball.* Thus the complementarity principle forbids superquantum configurations ($||\mathbf{r}||_2 > 1$), in the case of a qubit. This of course extends to arbitrary $d = 2^n$, since arbitrary states of many qubits are obtained through quantum operations (here at our disposal) over individual qubits. The conclusion is that for states of many qubits, superquantum configurations violate the complementarity principle by extension. We thus conclude that only one of the following assertives is true:

1. superquantum configurations exist in nature;

2. the complementarity principle is right.

Complementarity implies a fundamental bound on the possibilities beyond classical physics, a bound which coincides with quantum limits. However, it is known that even quantum computers have not indefinite power[10] [11]. The alternative paradigm is much more powerfull [14], but neverthless brings big conceptual complications [95].

2.4 Classicality criteria

In the previous section, many different formulations of classicality were given, based on quasiprobability representations of the states. In practice, however, determining whether an unknown state is nonclassical or not according to some definition is not an easy task. One would need to experimentally reconstruct the density matrix of the state, which is a highly demanding experimental procedure [96, 97]. Hence, criteria for determining the classicality directly from measurements and operations performed

[10]Unless it is shown that $P = NP$. But if this true, almost every problem is mostly trivial.

on the physical system are desirable[11]. The first procedure presented in what follows was developed by us [98] and gives an observable-based criteria of nonclassicality. It is based on a general definition of classicality, which will be shown later to be at least necessary in order to understand the task of entanglement creation described in the next chapter. Then we consider other important classicality criteria in the literature which are important for further sections.

2.4.1 Nonclassicality witnesses

The various definitions of classicality defined previously share a common structure: classical states are those expressed as convex combinations of extremal (pure) classical states, while nonclassical states are those which cannot be written in this fashion. Also, the pure classical states generally are complete or overcomplete basis of the state space and satisfy either a PVM or POVM relation. We thus define a *classical basis* $C = \{|c_\nu\rangle\}$ as a fixed basis of the Hilbert space $\mathcal{H}$ that describes the system at hand. This basis is choosen by physical reasons and can be continuous, discrete or mixed. It should be a resolution of identity $\int |c_\nu\rangle\langle c_\nu| d\mu(c_\nu) = I$, for some convenient fixed probability measure μ. The reasons to elect the classical basis C depend on the problem at hand and give the notion of classicality desired. For example, CCS are those that best mimic classical features in the quantum harmonic oscillator case. We arrive at the following definition of classicality relative to a classical basis:

Definition 4 *A state is classical relative to a classical basis C if it can be approximated in some operator norm[12] by states of the form*

$$\rho_c = \sum_i p_i |c_i\rangle\langle c_i| \tag{2.64}$$

with $\{p_i\}$ a probability distribution. Equivalently, ρ is classical if there exists a probability measure μ and a probability distribution P such that

$$\rho = \int_\Omega P(c)|c\rangle\langle c| d\mu(c) \tag{2.65}$$

[11] One should note that for an arbitrary unknown state some classicality criterion can demand the same amount of resources as the reconstruction task. In a practical situation, however, the experimentalist has some previous knowledge of the states that are achievable with the setup at hand. Then the criterion is invoked in order to certify the nonclassical character of his state.

[12] It is usual to take the trace norm in physics, due to technical advantages. Here we allow any operator norm, due to possible notions of classicality in other scenarios, e.g., numerical analysis or algorithmic ordering.

with Ω being the probability space considered in the context. Otherwise, the state is nonclassical in relation to the classical basis C.

This is an extension of the definition of separability for composite systems given in [99]. We see by the definition that the set of classical states is closed and convex. We use this to develop a method to detect the nonclassicality of a state in terms of observables available in a system.

Since the set of classical states is closed and convex by Definition 4, we can separate it from states that are outside the set, by using the following theorem, known as the Hahn-Banach separation theorem [100]:

Theorem 4 *Given two closed convex sets S_1 and S_2 in a real Banach space, one of which is compact, then there exists a bounded linear functional f and $\xi \in R$ such that $f(s_1) < \xi \leq f(s_2)$, for all $s_1 \in S_1$, $s_2 \in S_2$.*

The functional f can be uniquely represented in terms of an observable W as $f(\rho) = Tr(W\rho)$, with $W \in \mathcal{B}(\mathcal{H})$. This comes from the isomorphism between the space of bounded operators and the dual space of trace-class operators.

Lemma 1 *For every nonclassical state ρ_{nc}, there exists an observable W such that $Tr(W\rho_{nc}) < 0$ and $Tr(W\rho_c) \geq 0$, for all classical state ρ_c.*

Proof: The set of classical states is closed and convex. The same is true for the set $\{\rho_{nc}\}$, i.e., constituted of one point, which is also compact. From Theorem 2, we have that there exists $\tilde{W}$ and $\xi \in R$ such that

$$Tr(\tilde{W}\rho_{nc}) < \xi \leq Tr(\tilde{W}\rho_c) \tag{2.66}$$

for any classical ρ_c. Since $\xi = Tr(I\rho_{nc}\xi) = Tr(I\rho_c\xi)$, we define $W = \tilde{W} - \xi I$ and arrive at

$$Tr(W\rho_{nc}) < 0 \leq Tr(W\rho_c) \tag{2.67}$$

for all ρ_c, which proves the lemma, QED.

Employing the usual terminology of entanglement theory [103], we give the following definition

Definition 5 *A bounded hermitean operator W is a nonclassicality witness if $Tr(W\rho_c) \geq 0$ for every classical state ρ_c and there exists at least one nonclassical state ρ_{nc} such that $Tr(W\rho_{nc}) < 0$.*

The definition of a nonclassicality witness is not new, but is usually restricted to the context of quantum optics or specific quantum systems. The extension to general quantum systems is not superfluous, although obvious for the initiated, since it gives an equivalent way of *defining* nonclassicality in terms of observable quantities which does not invoke ontological modelations and/or quasiprobability distributions. Indeed, it will be shown that nonclassicality notions coming from quasiprobability distributions are too restrictive to capture the notion of nonclassicality induced by the task of entanglement creation in some physical systems. Thus, we get a consistent definition of nonclassicality for arbitrary quantum systems through the following equivalence:

Theorem 5 *A state ρ is classical iff $Tr(W\rho) \geq 0$ for all nonclassicality witnesses W.*

Proof: If ρ is classical then $Tr(W\rho) \geq 0$ by definition. If $Tr(W\rho) \geq 0$ for all nonclassicality witnesses W, let us suppose that ρ is nonclassical. By Lemma 1, there would exist a nonclassicality witness $\tilde{W}$ such that $Tr(\tilde{W}\rho) \geq 0$, which is a contradiction with the hypothesis. Thus, the theorem holds, QED.

Thus, classicality relative to a classical basis is equivalent to positivity under all nonclassicality witnesses relative to this basis. It is of course easier to detect the nonclassicality of a state, since this is implied by a negative mean value for one witness. Before entering in details, let us refine this result. We say that a witness W_1 is finer than a witness W_2 if W_1 detects all states detected by W_2 and some more states. The witness is optimal if no other witness is finer than it. Then we see that only optimal witnesses are needed in Theorem 5.

Construction of witnesses

Theorem 5 is not constructive, not presenting a method to design nonclassicality witnesses. Inspired by the methods in references [101, 102], we develop a method to construct witnesses from an arbitrary observable, which enables us to give a notion of which measurements are classical or not in an experiment. We present some examples of states detected by our method and also give conditions on the observables used to detect the nonclassicality notion associated to GCS.

Given a bounded hermitean operator M and a classical basis C, we define the following linear functional

$$\lambda(M) = \max_{|c\rangle \in C} \{\langle c|M|c\rangle : |c\rangle \in C\} \tag{2.68}$$

where the maximization is done over the classical basis C, which contains the extremal points of the convex set of classical states. So, we are taking some test observable M and looking for its maximal mean value over the set of classical states. The observable M in principle is arbitrary, but a nice motivation is to choose it among those that we have acess in practice. It can be also choosen by more abstract motivations as, e.g., observables whose $\lambda(M)$ is easy to calculate.

From the definition (2.68), we construct the following observable:

$$W_M = \lambda(M)I - M \tag{2.69}$$

which will be an optimal nonclassicality witness iff W_M has at least one negative eigenvalue, as is shown bellow. At least the eigenstate corresponding to this negative eigenvalue will be a nonclassical state, obviously.

Observation 3 *Observable (2.69) has positive mean value for any classical state.*

Proof: A classical state in relation to a classical basis C can be expressed as

$$\rho = \int_{\Omega} P(c)|c\rangle\langle c|d\mu(c) \tag{2.70}$$

for some probability distribution P and fixed probability space Ω and probability measure μ. Taking the mean value of M on this state and using the linearity of the trace, we have

$$\langle M\rangle = \int_{\Omega} P(c)\underbrace{\langle c|M|c\rangle}_{\leq\lambda(M)} d\mu(c) \leq \lambda(M) \tag{2.71}$$

implying that $Tr(W_M\rho) = \lambda(M) - Tr(M\rho) \geq 0$, QED.

Thus, if the mean value of W_M is negative for some state, the state is necessarilly nonclassical and we say that its nonclassicality is detected by the observable W_M. Let us see a simple condition on M such that W_M qualifies as a witness.

Lemma 2 *Observable (2.69) yields a usefull nonclassicality witness iff there exists at least one eigenvalue m of the observable M such that $\lambda(M) < m$.*

Proof: If there is an eigenvalue m of M such that $\lambda(M) < m$, let $|m\rangle$ be a eigenvector corresponding to this eigenvalue. Then $Tr(W_M|m\rangle\langle m|) = \lambda(M) - \langle m|M|m\rangle = \lambda(M) - m < 0$ and thus W_M is a nonclassicality witness, since by Observation 3 it has positive mean value for all classical states, while having negative mean value on the state $|m\rangle$.

This proves the backward claim. Now, for the forward claim, if W_M is a nonclassicality witness, then it has a negative value on some state. Let us suppose that $\lambda(M) \geq m$ for all eigenvalues of M. Then we have $\lambda(M) \geq \max_m\{m \in eigenvalue(M)\} \geq \langle\psi|M|\psi\rangle$, for every $|\psi\rangle$. The last inequality comes from the fact that the maximal mean value of an observable is given by its maximal eigenvalue [18]. This implies that W_M is a positive semidefinite operator, since $\langle\psi|W_M|\psi\rangle = \lambda(M) - \langle\psi|M|\psi\rangle \geq 0$, for every $|\psi\rangle$. But this is a contradiction with the hypothesis of W_M being a nonclassicality witness. Thus, the forward claim holds as well and the equivalence holds, QED.

We can then prove a general result for GCS:

Theorem 6 *If the dynamical symmetry group of a system is given by a compact semisimple Lie-group G, then observables in the associated Lie-algebra* g *are useless to detect nonclassicality associated to this symmetry.*

Proof: Let $M \in \mathsf{g}$. Then there exists a generalized coherent state $|\alpha_G\rangle$ such that $M|\alpha_G\rangle = m|\alpha_G\rangle$ and m is a maximal eigenvalue of M (highest weight). Since the maximal eigenvalue of an operator is the maximal mean value of this operator, we have $\lambda(M) = m$ and there is not an eigenvalue m' of M such that $\lambda(M) < m'$. By Lemma 2, the witness constructed from M is useless to detect any nonclassicality associated to G, QED.

The interpretation of this result is that observables sharing the symmetry of the system are "blind" to nonclassical effects beyond this symmetry. Thus, any such nonclassical effect will appear as "magical" for observers constrained to the dynamical symmetry group of the system. This, however, does not imply an impossibility of detecting the nonclassicality with generators. The mean value of an observable $M \notin \mathsf{g}$ can in many cases be infered from the mean values of a collection of generators.

Finally, for completeness, one can extend the result in [102] to nonclassicality witnesses:

Theorem 7 *An arbitrary nonclassicality witness W can be expressed in the form (2.69).*

The demonstrations in [102] do not rely on the composite nature of the state space, thus they extend naturally to arbitrary convex definitions of classicality.

Example 1: $SU(2)$ coherent states

For a classical basis constituted of $SU(2)$ coherent states, the generators of the Lie-algebra $\mathsf{su}(2)$ are given by the angular momentum operators $J_n \equiv \mathbf{J}\cdot\mathbf{n}$, as is well-known. The witnesses constructed from these observables by (2.69) will not give any information, as concluded in Theorem 6. We must consider the mean values of higher order terms such as $(J_x)^2, J_xJ_y, J_xJ_z, (J_y)^2, \ldots$, in order to construct usefull nonclassicality witnesses. Although it can be hard to design apparatuses to implement these higher order observables, one can obtain their mean values (multipolar moments) as described in [104]. The higher order moments are related to the moments of J_n in different directions $\mathbf{n}$ through a system of linear equations. The price paid for such simplification is that the system of equations is generally redundant and the number of different directions to be measured can grow quickly with increasing number of particles. When dealing with Stern-Gerlach apparatuses, a perhaps easier alternative is to consider Feynman filters [105]. The idea is that an arbitrary rank-one projector is the eigenstate of some J_n. The examples of observables considered here are all rank-one projectors, so one would need simply to find the proper direction $\mathbf{n}$ and record the rate at which the detector in this direction is hit; rates at other directions should be discarded, or used to infer mean values of higher-rank observables.

Let us consider a spin-1 particle. The basis of the three-dimensional Hilbert space is $\{|-1\rangle, |0\rangle, |1\rangle\}$ and the angular momentum operators are given by

$$J_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \quad J_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}; \quad J_z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2.72}$$

The $SU(2)$ coherent states are given by expression (1.12), which in this case simplifies to

$$|z\rangle = \left(\frac{1}{1+|z|^2}\right)(|-1\rangle + z\sqrt{2}|0\rangle + z^2|1\rangle) \tag{2.73}$$

Let us consider the quadrupole operator

$$M = (J_x)^2 - (J_y)^2 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{2.74}$$

which have as eigenvectors $|\psi_\pm\rangle = (1/\sqrt{2})(|-1\rangle \pm |1\rangle)$. Calculating its mean value on an arbitrary coherent state, we have

$$\langle z|M|z\rangle = \frac{2(z_r^2 - z_i^2)}{(1 + z_r^2 + z_i^2)^2} \tag{2.75}$$

implying that $\lambda(M) = 1/2$. The corresponding witness operator is

$$W_M = \lambda(M)I - M = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \tag{2.76}$$

and we get that $Tr(W_M|\psi_+\rangle\langle\psi_+|) = -1/2$, i.e., the state $|\psi_+\rangle$ is nonclassical. Also, the state

$$\rho = \frac{p}{3}I + (1-p)|\psi_+\rangle\langle\psi_+| \tag{2.77}$$

obeys $Tr(W_M\rho) = p - 1/2$ and thus the nonclassicality of ρ is detected whenever $p < 1/2$.

Example 2: d-level systems

In the case where one chooses the classical basis as the computational basis $C = \{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$, then the classical states have the simple form $\rho_c = \sum_k p_k|k\rangle\langle k|$. Thus, any superposition of states of the classical basis is nonclassical. To see this, we take a generic state $|\psi\rangle = \sum_{i=0}^{d-1} c_i|i\rangle$. Then, we just need to consider the observable $M_\psi = |\psi\rangle\langle\psi|$. The functional $\lambda(M_\psi) = \max_k\{\langle k|M_\psi|k\rangle\} = \max_k\{|c_k|^2\}$ implies that $Tr(W_{M_\psi}|\psi\rangle\langle\psi|) = \max_k\{|c_k|^2\} - 1$ is nonnegative iff $\max_k\{|c_k|^2\} = 1$, i.e., iff $|\psi\rangle$ is a member of the computational basis C. This observation can be extended to mixed states as well [98].

Example 3: the qubit case

Let us compare the two previous examples of classicality notions for a qubit. In this situation, every pure state is an eigenstate of a matrix $\sigma \cdot \mathbf{n}$. Thus, every pure state is a $SU(2)$ coherent state, which can be seen also from the formula (1.12)

$$|z\rangle = \left(\frac{1}{1+|z|^2}\right)(|0\rangle + z|1\rangle) \tag{2.78}$$

But, since every mixed state of a qubit is a convex combination of two pure qubit states, every mixed state is classical as well. Hence, in relation to the classical basis of $SU(2)$ coherent states, every qubit is classical.

The situation is radically different when the classical basis is the computational basis $C = \{|0\rangle, |1\rangle\}$. Then the classical states are of the form $\rho_c = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|$, which in the Bloch picture is simply

$$\rho_c = \frac{1}{2}[I + (2p-1)\sigma_z] \tag{2.79}$$

implying that the classical states all lie in the z axis of the Bloch ball, which is a null-measure set. Thus, for the notion of classicality related to the computational basis, almost all states are nonclassical.

2.4.2 Matrix of moments criterion

In [106, 107], Shchukin, Richter and Vogel derived a practical and very strong criterion that determines the P-representability of a state in terms of matrices formed by moments of creation and annihilation operators in normal order. Since these moments have clear operational significance in terms of experimental procedures related to homodyne detection, it is in principle possible to completely characterize the nonclassicality associated to P-representability. We need the following result, known as Bochner's Theorem [108]:

Theorem 8 *The Glauber-Sudarshan distribution is a genuine probability distribution on the complex plane iff for any smooth distribution f with compact support the following expression is nonnegative:*

$$\int\int \xi(\alpha-\beta) f^*(\alpha) f(\beta) d^2\alpha d^2\beta \geq 0 \tag{2.80}$$

where ξ is the characteristic function of the P distribution:

$$\xi(\beta) = \int P(\alpha) e^{\alpha\beta^* - \alpha^*\beta} d^2\alpha \tag{2.81}$$

The equivalence between P-representability and positivity conditions on the characteristic function ξ can be translated in terms of positivity in operator form. To this end, let us define the following infinite dimensional matrix of moments:

$$M = \begin{pmatrix} 1 & \langle a\rangle & \langle a^\dagger\rangle & \langle a^2\rangle & \langle a^\dagger a\rangle & \langle (a^\dagger)^2\rangle & \dots \\ \langle a^\dagger\rangle & \langle a^\dagger a\rangle & \langle (a^\dagger)^2\rangle & \langle a^\dagger a^2\rangle & \langle (a^\dagger)^2 a\rangle & \langle (a^\dagger)^3\rangle & \dots \\ \langle a\rangle & \langle a^2\rangle & \langle a^\dagger a\rangle & \langle a^3\rangle & \langle a^\dagger a^2\rangle & \langle (a^\dagger)^2 a\rangle & \dots \\ \langle (a^\dagger)^2\rangle & \langle (a^\dagger)^2 a\rangle & \langle (a^\dagger)^3\rangle & \langle (a^\dagger)^2 a^2\rangle & \langle (a^\dagger)^3 a\rangle & \langle (a^\dagger)^4\rangle & \dots \\ \langle a^\dagger a\rangle & \langle a^\dagger a^2\rangle & \langle (a^\dagger)^2 a\rangle & \langle a^\dagger a^3\rangle & \langle (a^\dagger)^2 a^2\rangle & \langle (a^\dagger)^3 a\rangle & \dots \\ \langle a^2\rangle & a^3 & \langle a^\dagger a^2\rangle & \langle a^4\rangle & \langle a^\dagger a^3\rangle & \langle (a^\dagger)^2 a^2\rangle & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{2.82}$$

Bochner's Theorem can be rewritten then in the following form:

Theorem 9 *A state is P-representable iff M is positive semidefinite.*

Since a matrix is positive semidefinite iff all its principal minors are nonnegative, a negative eigenvalue in any principal minor implies a nonclassical state. This is a considerable practical improvement, since it gives a criterion that can be observed experimentally through measurements of the normally-ordered moments $\langle (a^\dagger)^m a^n \rangle$, which can be observed by well-known techniques of homodyne detection. Moreover, the test associated to a particular minor can be seen as a nonlinear nonclassicality witness, since it is a functional relation positive for all classical states and is negative for some nonclassical states.

2.4.3 Rivas-Luis criterion

In [4], Rivas and Luis developed a criterion of P-representability (GCS included) based on the statistical behaviour of a measurement. The parallels with our criterion are many, representing a different point of view on nonclassicality. As saw previously, in the GCS picture a state admits a P-representation (2.21)

$$\rho = \int P(\alpha_G) |\alpha_G\rangle\langle\alpha_G| d\mu(\alpha_G). \tag{2.83}$$

Then it is straightforward to check that

$$Tr(M\rho) = \int P(\alpha_G) Q_M(\alpha_G) d\mu(\alpha_G), \tag{2.84}$$

where $Q_M(\alpha_G)$ is the Husimi distribution (2.22) of the operator M. Writing $\lambda_M = \max\{Q_M(\alpha_G)\}$, we have $P(\alpha_G)Q_M(\alpha_G) \leq P(\alpha_G)\lambda_M$, whenever $P(\alpha_G)$ is a true probability distribution, i.e., the state is classical. Then we must have

$$Tr(M\rho) \leq \lambda_M \int P(\alpha_G) d\mu(\alpha_G) = \lambda_M \tag{2.85}$$

and thus ordinary classical statistics demands that

$$Tr(M\rho) \leq \lambda_M \tag{2.86}$$

In [4], the operator M is a member of a general POVM. There are many states that violate this statistical bound and in this sense these states are nonclassical.

If we consider M as an observable, we see that λ_M is just the functional (2.68) when the classical basis is composed of GCS. In this situation, our criterion is identical to the Rivas-Luis criterion. Or, in other words, Rivas-Luis criterion can be seen as a nonclassicality witness test. Our criterion can be extended to more exotic notions of nonclassicality, since it does not rely on implicit quasiprobability distributions constructions, as the criterion of Rivas and Luis. However, Rivas-Luis criterion can also be formulated to establish a statistical criterion of classicality of a measurement, while our criterion implicitly identifies the nonclassicality of a measurement by its usefullness as a nonclassicality witness.

Chapter 3

Entanglement

"One concept corrupts and confuses the others. I am not speaking of the Evil whose limited sphere is ethics; I am speaking of the infinite."
Jorge Luis Borges

3.1 Definitions

The name *entanglement* was coined by Schrödinger [2] shortly after the appearance of the EPR paradox [59], in order to give a better understanding of the radical implications of quantum mechanics[1]. For Schrödinger, entanglement was *the* characteristic trait of quantum physics. Since in that time the definition of mixed states did not exist yet, there was a certain vague identification of entanglement and nonlocality, which persisted for many decades. The formal definition of entanglement is due to Werner [99], separating the concepts of locality and separability of correlations, which were previously considered on the same footing.

Definition 6 *A state $\rho \in \mathcal{B}(\mathcal{H})$ is separable if it can be approximated in the trace-norm[2] by convex combinations of product-states, i.e.,*

$$\rho_s = \sum_i p_i \rho_i^A \otimes \rho_i^B \tag{3.1}$$

with $\rho_i^k \in \mathcal{B}(\mathcal{H}_k)$ and $\{p_i\}$ a probability distribution - $p_i \geq 0$ and $\sum_i p_i = 1$. Otherwise, we say that the state is inseparable or entangled.

[1]The practical applications of entanglement and nonlocality are very powerfull and varied. The interested reader can consult the references [6, 7, 9] for a survey.

[2]This demand makes the set of separable states closed under the trace-norm. This is relevant for infinite-dimensional systems.

Considering the local observable $M = M_A \otimes M_B$, with $M_A \in \mathcal{H}_A$ and $M_B \in \mathcal{H}_B$, we see that its mean value for a separable state ρ_s is approximated by

$$\langle M \rangle_s = \sum_i p_i Tr(M_A \rho_i^A) Tr(M_B \rho_i^B) = \sum_i p_i \langle M_A \rangle_i \langle M_B \rangle_i, \tag{3.2}$$

with obvious notation. Thus the mean value of a local observable on a separable state is given by the rules of standard probability theory for composite systems displaying a correlation. This correlation is classical in the sense that we do not have to invoke quantum theory to explain it: a separable state is statistically indistinguishable from one in which the i-th local states $\rho_i^A \otimes \rho_i^B$ are locally prepared according to the result of a common random number generator which gives number i with probability p_i. For pure states, the definition specializes to

Definition 7 *A pure state $|\psi\rangle \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ is separable if it can be decomposed as a product-state, i.e,*

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \tag{3.3}$$

with $|\psi_i\rangle \in \mathcal{H}_i$. Otherwise, the state is entangled.

In this special situation, entanglement is equivalent to nonlocality [109]. It is easy to see that product-states $\rho_A \otimes \rho_B$ (not only pure ones) described systems that are totally uncorrelated. Taking once again the local observable $M = M_A \otimes M_B$, we see that its mean value on a product-state is given by $\langle M \rangle = \langle M_A \rangle \langle M_B \rangle$, i.e., the measurements are uncorrelated.

The extensions to the multipartite case are straightforward, but there are some subtleties. For a composite system $\mathcal{H} = \bigotimes_i \mathcal{H}_i$, we have

Definition 8 *A state is separable if it can be approximated by*

$$\rho_s = \sum_i p_i \bigotimes_j \rho_i^j \tag{3.4}$$

where $\rho_i^k \in \mathcal{B}(\mathcal{H}_k)$ and $\{p_i\}$ is a probability distribution.

In some situations extra care is needed in order to address the problem correctly. For example, in a tripartite system $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, one can consider the separability in relation to the full tripartition, or, defining $\mathcal{H}_D = \mathcal{H}_B \otimes \mathcal{H}_C$, one could consider the separability in relation to the bipartition $\mathcal{H}_A \otimes \mathcal{H}_D$, or any other bipartition.

3.2 Separability criteria

The direct determination of separability of an arbitrary density matrix is a problem of high computational complexity [110, 111]. Moreover, the experimental reconstruction of an arbitrary preparation consumes a number of resources that increases exponentailly with the system dimension [96, 97]. Hence, there is a practical need of detecting directly the entanglement of a state through separability criteria that do not demand the whole knowledge of the density matrix of a preparation. There exists many non-equivalent separability criteria in the literature [9, 112] and we will then present here the most relevant for the results in this thesis.

3.2.1 Horodecki's criterion

We describe here the two equivalent formulations of the Horodecki's Criterion [117], which is a necessary and sufficient separability criterion and is the most important one in entanglement theory.

Entanglement witnesses

The great number of articles related to the so-called witnesses was fostered by the successes and many applications in entanglement theory. We review quickly the main definitions and theorems in case the reader skipped the chapter on nonclassicality.

Definition 9 *An observable $W \in \mathcal{B}(\mathcal{H}_A) \otimes \mathcal{B}(\mathcal{H}_B)$ is an entanglement witness if*

- $Tr(W\rho_s) \geq 0$*, for every separable state* ρ_s*;*
- *There exists at least one entangled state* ρ_e *such that* $Tr(W\rho_e) < 0$*.*

Although the definition appears originally in [117], the name "entanglement witness" was coined by Terhal in [103], where the importance of the concept and the potential applications in entanglement and nonlocality detection were highlighted. From this definition, one obtains the following necessary and sufficient separability criterion:

Theorem 10 *A state ρ is separable iff $Tr(W\rho) \geq 0$ for every entanglement witness W.*

In other words, if there exists a witness with negative mean value for some state, then this state is entangled. Before proving the theorem, we need to prove the following lemma:

Lemma 3 *For every entangled state ρ_e, there exists an entanglement witness W which detects its entanglement, i.e., there exists a witness W such that $Tr(W\rho_e) < 0$.*

Proof of the Lemma: The same as Lemma 1, taking the set of classical states as pure product states, QED.
Proof of the Theorem: The same as Theorem 5, taking the set of classical states as pure product states, QED.

Although general, the Theorem above is not constructive, since we do not know which observable we should measure in order to detect the entanglement of a given state. In [101, 102], a way of constructing witnesses from observables available in practice was obtained; also, this technique has a great practical appeal and is not limited to entanglement theory and we thus extended it to arbitrary (convex) definitions of nonclassicality in the previous chapter. Given an observable $M \in \mathcal{B}(\mathcal{H}_A) \otimes \mathcal{B}(\mathcal{H}_B)$, one defines the following linear functional

$$\lambda(M) = \max_{|\psi_A\rangle\otimes|\phi_B\rangle\in\mathcal{H}} \langle\psi_A, \phi_B|M|\psi_A, \phi_B\rangle \tag{3.5}$$

where the maximization is done over the set of pure product states[3]. From this definition, we have that the following observable is an optimal entanglement witness[4]:

$$W_M = \lambda(M)I - M \tag{3.6}$$

In [102], the generality of this method was proven. Also, it was developed a method of finding this optimal value through so-called separability eigenvalue equations.

The construction (3.5) enabled the experimental detection in different setups, mainly taking the Hamiltonian H as the test observable. In some models of spin chains, for example, the calculation of $\lambda(H)$ is easy to perform or approximate. Then one can detect entanglement using energy measurements [101, 118], establishing connections between thermodynamical quantities in condensed matter models and entanglement properties [119]. More examples and similar approaches based on witnesses can be found in [112]. This broad range of applications was one of the main motivations to propose the extension of witnesses to general notions of classicality considered in the previous chapter.

[3] Which are the extremal points of the set of separable states and thus any separable state can be written as a convex combination of pure product states. This can be seen also from the definition of a separable state, since it is just a matter of writing the spectral decomposition of the local states in the decomposition (3.1).

[4] Optimal in the sense that there not exists another witness that detects more states than it. See also the discussion in the paragraph bellow Theorem 5.

Positive maps

We can reformulate Theorem 10 in the language of positive maps, establishing an equivalence between two mathematical problems of enormous relevance and difficulty. The main idea is to use the well-known [120] isomorphism between the space $\mathcal{M}^* \otimes \mathcal{N}$ and the linear maps of $\mathcal{M}$ in $\mathcal{N}$. There are many isomorphisms at our disposal, but one particularly make explicit the connection between positive maps and entanglement witnesses, giving an elegant general vision of the problem and creating certain intuition on how to handle some tractable cases. This special isomorphism is given by

$$\Lambda(\rho) = Tr_B(M\rho^T \otimes I_B) \tag{3.7}$$

with inverse isomorphism

$$M = (I_A \otimes \Lambda)(|\phi_d^+\rangle\langle\phi_d^+|) \tag{3.8}$$

This isomorphism is known in the literature as Choi-Jamiolkowski Isomorphism [121, 122], although its originality being disputed [123]. This transformation takes an observable $M \in \mathcal{B}(\mathcal{H}_A) \otimes \mathcal{B}(\mathcal{H}_B)$ in a linear map $\Lambda \in \mathcal{L}(\mathcal{B}(\mathcal{H}_A), \mathcal{B}(\mathcal{H}_B))$. This map is CP (see definitions in Section 1.4.) iff M is positive semidefinite and NCP iff M is an entanglement witness. From this last observation, we obtain the following equivalent formulation of the Horodecki's Criterion:

Theorem 11 *A state ρ is separable iff $I_A \otimes \Lambda(\rho) \geq 0$ for all positive map Λ.*

The only relevant maps for the detection of entanglement are clearly the NCP maps. Hence Horodecki's Criterion establishes an equivalence between the separability problem and the old open problem of classification of NCP maps [19, 9]. It is noteworthy that individually a NCP map is more powerfull in detecting entanglement than an entanglement witness, since the condition given by a witness is of scalar type, while that given by a map is of operator type. But from a practical point of view, witnesses are observables that can be readilly implementated or estimated, while NCP maps are not directly implementable in a laboratory, since quantum operations of an isolated system are CP maps.

3.2.2 Peres' criterion

The simplest and most important example of a NCP map is the transposition T, which maps $|i\rangle\langle j|$ to $|j\rangle\langle i|$. It is positive since it does not change the eigenvalues of an operator

[18], but NCP, as can be verified for the matrix $|\phi\rangle\langle\phi|$, with $|\phi\rangle = |00\rangle + |11\rangle$ when acted by $I_A \otimes T_B$. This last transformation is known as *partial transposition.* In terms of the orthonormal basis $\{|e_m\rangle\}_{m=0}^{d_A}$ of $\mathcal{H}_A$ and $\{|f_n\rangle\}_{n=0}^{d_B}$ of $\mathcal{H}_B$, we apply the following transformation to the elements of the density matrix $\rho_{\mu\alpha\eta\beta} = \langle e_\mu \otimes f_\alpha|\rho|e_\eta \otimes f_\beta\rangle$ of an arbitrary state $\rho \in \mathcal{B}(\mathcal{H}) = \mathcal{B}(\mathcal{H}_A) \otimes \mathcal{B}(\mathcal{H}_B)$:

$$\langle e_\mu \otimes f_\alpha|\rho^{T_B}|e_\eta \otimes f_\beta\rangle = \langle e_\mu \otimes f_\beta|\rho|e_\eta \otimes f_\alpha\rangle = \rho_{\mu\beta\eta\alpha}$$

This transformation corresponds to performing the transposition only on the matrix elements corresponding to the second subsystem, i.e., to apply the transformation $I_A \otimes T_B$, where I_A is the identity operation in the first subsystem and T_B is the transposition operation in the second subsystem.

Considering a separable state $\rho_s = \sum_i p_i \rho_A^i \otimes \rho_B^i$, the partial transposition matrix is simply

$$\rho^{T_B} = (I_A \otimes T_B)\rho_s = \sum_i p_i \rho_A^i \otimes (\rho_B^i)^T$$

Since the transposition preserves the trace, eigenvalues and hermiticity of the various ρ_B^i, we see that $(\rho_B^i)^T$ represents a state and hence ρ^{T_B} also corresponds to a state. Thus, we arrive at the following necessary condition for separability [124]:

Theorem 12 *If ρ is a separable state, then its partial transposition is a state as well.*

Thus, given an arbitrary state, if its partial tranposition does not corresponds to a state, one concludes that this state is entangled. It is enough to just check the presence of a negative eigenvalue in the partial transposition, since this operation does not change the trace or hermiticity of the global state. In [125], a nice physical interpretation of the partial transposition in terms of the time reversal symmetry was given. The idea is that for Hermitean matrices the transposition map corresponds to the complex conjugation operation K. Since the time reversal operation Θ is unitarilly equivalent to the conjugation operation, i.e., there exists an unitary U such that $\Theta = UK$, the partial transposition is equivalent to a local time reversal operation. Then what Peres' Criterion roughly means is that the set of separable states is invariant under local changes of time direction. A nice description of this relationship for two and many qubits is given by [126].

The transposition map is an example of *Co-Completely Positive* (CoCP) map, which is a map that when composed with tranposition yields a CP map. As proved by [127, 128], if the subsystem's dimensions satisfy $d_A d_B \leq 6$, all positive maps are convex combinations of CP maps and CoCP maps:

$$\Lambda = a\Lambda_{CP} + (1-a)\Lambda_{CoCP} \tag{3.9}$$

A map that admits the above decomposition is called *decomposable*. Thus, if the global system has a maximal dimension of 6, all maps are decomposable, implying the following theorem, known as Peres-Horodecki Theorem [117, 124]:

Theorem 13 *For a $2\otimes 2$ system (two qubits) or a $2\otimes 3$ system (a qubit and a qutrit), Peres' Criterion is also sufficient for the separability of a state.*

Proof: For these two cases, all positive maps are decomposable, and thus a state that is positive under partial transposition is positive for all positive maps; by Horodecki's Criterion, this implies that the state is separable, QED.

For higher dimensions there are states which satisfy Peres' Criterion, i.e., that are Positive under Partial Transposition (PPT) and are also entangled. The maps used to detect this kind of entanglement should obviously be at least *indecomposable*, i.e., not of the form (3.9). We will call these states PPT entangled states; they are one of the central topics of this thesis, as will be clear in further sections. It is important to notice that the Peres-Horodecki Theorem does not exhausts all states for which Peres' Criterion is sufficient. PPT states are separable whenever the rank of the state is sufficiently low [130], for highly symmetric states [99, 129], Gaussian states [131, 116], a special class of states in continuous variables [113] and, as proved by us in [132], for states in arbitrary dimensions with a special block structure which does not relate to any notion of small dimensionality.

3.2.3 Range criterion

A criterion independent from Peres' Criterion is the so-called *Range Criterion*[5] [133], whose general formulation is the following:

Theorem 14 *Given a separable state ρ_s, there exists a set of product-vectors $\{|a_i, b_j\rangle\}$ which spans $Range(\rho)$ and such that $\{|a_i, b_j^*\rangle\}$ spans $Range(\rho^{T_B})$.*

[5] The range of a matrix M is the set $Range(M) = \{|\psi\rangle \in \mathcal{H} : M|\phi\rangle = |\psi\rangle$,for some $|\phi\rangle \in \mathcal{H}\}$.

A simple way of using this criterion to construct PPT entangled states is through *Unextendible Product Basis* (UPB) [134], which is a basis with pairwise orthogonal elements and such that no other product-vector is orthogonal to this set. An example for a $3 \otimes 3$ system is the basis

$$\begin{aligned} |\psi_0\rangle &= \frac{1}{\sqrt{2}}|0\rangle(|0\rangle - |1\rangle); \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)|2\rangle; \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}|2\rangle(|1\rangle - |2\rangle); \\ |\psi_3\rangle &= \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)|0\rangle; \quad |\psi_4\rangle = \frac{1}{3}(|0\rangle + |1\rangle + |2\rangle)(|0\rangle + |1\rangle + |2\rangle) \end{aligned}$$

Thus, defining the state

$$\rho_{upb} = \frac{1}{4}\left(I - \sum_{i=0}^{4} |\psi_i\rangle\langle\psi_i|\right) \tag{3.10}$$

we see that there is no vector-product in its range and thus the state is entangled. As $\rho_{upb} = \rho_{upb}^{T_B}$, the state is PPT entangled. Other examples of PPT entanglement detected by the Range Criterion are given in [133, 139, 115] and the novel class of states that we will construct in further sections.

3.3 Entanglement creation

Entanglement is a nonclassical phenomenom of central importance in quantum information protocols and hence understanding how to generate this resource is almost obligatory. Most discussions in this direction concentrate on the generation of entanglement in a particular physical system: take the eigenstates of some Hamiltonian, find some pure entangled state (or apply some entanglement measure to detect some entanglement) and then analyse temporal evolution of the system. Albeit its relevance, such approaches are very poor from a theoretical point of view. It is desirable to understand what is the source of this radical nonclassical phenomenon in a general context, so that more conclusions can be draw independently of the representations associated to a system.

In this vein, a result from Asboth *et al* [135] shed some light on the central role of P-representability for entanglement creation in optical setups[6]. Given a one-mode state of the radiation ρ, one considers what happens when using this state as an input in a beam-splitter (BS), i.e., applying the unitary

$$U(\theta)\begin{pmatrix} {a_A}^\dagger \\ {a_B}^\dagger \end{pmatrix} = \begin{pmatrix} cos(\theta) & sin(\theta) \\ -sin(\theta) & cos(\theta) \end{pmatrix}\begin{pmatrix} {a_A}^\dagger \\ {a_B}^\dagger \end{pmatrix}, \tag{3.11}$$

[6]Other works with similar ideas can be found in [136, 137]

to a state $\rho_{in} = \rho \otimes |0\rangle\langle 0|$, producing the two-mode output state $\rho_{out} = U(\theta)\rho_{in}U^{\dagger}(\theta)$. The BS is a passive device, so any correlation observed in ρ_{out} is due solely to the one-mode state ρ. The authors in [135] establish an equivalence between the classicality of ρ and the separability of ρ_{out}:

Theorem 15 *The state ρ_{out} is separable iff ρ is P-representable.*

Hence, nonclassical light is an essencial resource in order to create entanglement in quantum optics. A similar situation arises in discrete systems, where the interaction analogous to the BS is given by the gate known as Controlled-NOT (CNOT), whose action on the computational basis is given by:

$$U_{CNOT}|i, j\rangle = |i, j \oplus_d i\rangle \tag{3.12}$$

Here d is the system's dimension and $\oplus_d$ represents summation modulo d. If, in analogy to the continuous case, we take an input state $\rho_{in} = \rho \otimes |0\rangle\langle 0|$, it is then possible to prove[7] the following result holds

Theorem 16 *The state $\rho_{out} = U_{CNOT}\rho_{in}U^{\dagger}_{CNOT}$ is separable iff $\rho = \sum_{i=0}^{d-1} p_i|i\rangle\langle i|$.*

Proof: If $\rho = \sum_{i=0}^{d-1} p_i|i\rangle\langle i|$, then $\rho_{out} = \sum_i p_i|i\rangle\langle i| \otimes |i\rangle\langle i|$ and the state is separable. Now, if the output state $\rho_{out} = U_{CNOT}\rho_{in}U^{\dagger}_{CNOT}$ is separable, then we have

$$\begin{aligned}
U_{CNOT}\rho_{in}U^{\dagger}_{CNOT} &= \sum_i p_i|\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i| && (3.13)\\
\Rightarrow \rho_{in} &= \sum_i p_i U^{\dagger}_{CNOT}(|\psi_i\rangle\langle\psi_i| \otimes |\phi_i\rangle\langle\phi_i|)U_{CNOT} && (3.14)\\
&= \sum_i p_i|i\rangle\langle i| \otimes |0\rangle\langle 0| && (3.15)
\end{aligned}$$

In the last step, we used the fact that a output state in the form $\rho_{out} = \sum_k p_k|\Psi_k\rangle\langle\Psi_k|$ resulting from an input $\rho_{in} \otimes |0\rangle\langle 0|$ should be consistent term-by-term, i.e., we should have $U^{\dagger}_{CNOT}|\Psi_k\rangle\langle\Psi_k|U_{CNOT} = |\xi_k\rangle \otimes |0\rangle$, for some $|\xi_k\rangle$. The only way to fulfill this requirement in the last step above is for states in the computational basis. Thus, a separable ρ_{out} implies $\rho = \sum_{i=0}^{d-1} p_i|i\rangle\langle i|$, QED.

As we have seen previously, states in the form $\rho = \sum_{i=0}^{d-1} p_i|i\rangle\langle i|$ are classical in relation to the computational basis, by Definition 4. In other words, the CNOT interaction *induces* the classicality notion given by the computational basis as the

[7]We do not know whether this result was already proven in another reference.

classical basis. Nonclassicality in this sense is once again the fundamental resource for entanglement creation in discrete systems. We stress that the CNOT operation is a fundamental gate in most proposals of quantum computation schemes [6, 7] and the indetification of the correct nonclassicality notion associated to this interaction have a big relevance[8].

Controlled displacements

The CNOT and BS interactions can be seen as Controlled Displacements (CD) in their respectives classical basis. Let us start with the BS. Without loss of genrality, we will consider a $50 : 50$ BS, i.e., $\theta = \pi/4$. The action of a $50 : 50$ BS in a pair of coherent states is given by

$$U(\pi/4)|\alpha,\beta\rangle = U(\pi/4)D_1(\alpha)D_2(\beta)|0,0\rangle = D_1\left(\frac{\alpha-\beta}{\sqrt{2}}\right)D_2\left(\frac{\alpha+\beta}{\sqrt{2}}\right)|0,0\rangle \quad (3.16)$$

where the subscripts refers to the local modes 1 and 2. If the second mode is in the vaccum state, we have

$$U(\pi/4)|\alpha,0\rangle = |\alpha/\sqrt{2},\alpha/\sqrt{2}\rangle \quad (3.17)$$

In terms of the displacement operators, this can be seen as the following transformation

$$D_1(\alpha)D_2(0) \to D_1(\alpha/\sqrt{2})D_2(\alpha/\sqrt{2}) \quad (3.18)$$

which is a structure of a controlled operation: the amount of displacement in the first (control) mode will determine the displacement of the second (target) mode; thus the BS is a kind of CD. For the CNOT the situation is similar, since we have

$$U_{CNOT}T_1(0,i)\otimes T_2(0,0)|0,0\rangle = |i,i\rangle = T_1(0,i)\otimes T_2(0,i)|0,0\rangle \quad (3.19)$$

where the discrete displacement $T(a,b)$ is defined in (1.17). In terms of transformations of the displacement operators we have

$$T_1(0,i)\otimes T_2(0,0) \to T_1(0,i)\otimes T_2(0,i) \quad (3.20)$$

once again a CD relation.

[8] A different approach related to the creation of multipartite entanglement using the CNOT is given by some works from Piani *et. al.* [138]. I am very thankfull to M. Piani for the many interesting comments and suggestions concerning [98].

Motivated by this, we define a general CD operation in relation to a classical basis $C = \{c_\mu\}$ as any unitary that performs the following map between the displacements in the classical basis[9]:

$$D_1(c_i)D_2(c_0) \rightarrow D_1(c_i)D_2(c_i) \tag{3.21}$$

With this definition, similar results to theorems 15 and 16 can be proven in arbitrary systems [98], provided this operation can be defined in the desired system. So, for example, let us analyse the classicality in relation to the $SU(2)$ symmetry and let us suppose that some unitary has the following effect on the $SU(2)$ displacement (1.11):

$$D_1(z)D_2(0)|j,j\rangle \rightarrow D_1(z)D_2(z)|j,j\rangle \tag{3.22}$$

Then, for example, the nonclassical state for a qutrit $|\psi_+\rangle = (1/\sqrt{2})(|-1\rangle + |+1\rangle)$ is mapped into

$$\begin{aligned} |\psi_+\rangle &= \frac{1}{\sqrt{2}}(D_1(\infty)D_2(0) + D_1(0)D_2(0))|+1,+1\rangle & (3.23)\\ \rightarrow |\Psi_+\rangle &= \frac{1}{\sqrt{2}}(D_1(\infty)D_2(\infty) + D_1(0)D_2(0))|+1,+1\rangle & (3.24)\\ \Rightarrow |\Psi_+\rangle &= \frac{1}{\sqrt{2}}(|-1,-1\rangle + |+1,+1\rangle) & (3.25) \end{aligned}$$

and the state is entangled, as expected.

On the necessity of Definition 4

From Theorem 16, we see that the nonclassicality associated to the computational basis is the resource for entanglement creation by the CNOT. However, a classical state in this sense has the form $\rho = \sum_i p_i |i\rangle\langle i|$. This is far from a quasiprobability distribution, since the computational basis is not informationally complete. We cannot, for example, perform a tomography of the state only using measurements in the classical basis. This is enough to show that quasiprobability distributions cannot fully describe the nonclassicality associated to entanglement creation. Hence, Definition 4 is at least necessary to understand quantum tasks that are beyond classical physics.

For completeness, let us give a trivial example closer to home. First, notice that the CNOT can be written as

$$U_{CNOT} = \sum_{k=0}^{d-1} |k\rangle\langle k| \otimes X^k \tag{3.26}$$

[9] The definition of displacements are obvious: they are simply permutations between the classical basis elements.

If we define another unitary by

$$U = \sum_{k\ even} |k\rangle\langle k| \otimes I + \sum_{k\ odd} |k\rangle\langle k| \otimes X^k \tag{3.27}$$

we see that any state that is a superposition of even states in the computational basis, $|\psi\rangle = \sum_m c_m|2m\rangle$ will generate no entanglement when we perform $U|\psi\rangle|0\rangle$. If we take the Fock basis as our computational basis, this would mean that the whole set vaccum-squeezed states, which are superpositions of even number states, would generate no entanglement and would be members of the classical basis. The subspace spanned by even number states is obviously not informationally complete and the nonclassicality notion would have no relation to any quasiprobability distribution. Thus, trying to understand how entanglement is generated with quasiprobability representations would be misleading.

3.4 Bound entanglement

The great appeal of entangled states comes from the possibility of generating any quantum state by the consumption of a finite number of singlet states and manipulation via LOCC, which are deterministic and noiseless procedures. This can be accomplished through a protocol known as *entanglement dilution* [140], given that a sample of pure (maximally entangled) states is diluted by LOCC and generates some copies of a desired state. This estimulated a large number of proposals for the generation of maximally entangled pure states, since if one can prepare many copies of such states, then any quantum channel is implementable by dilution. However, pure states are mostly an abstraction, since it is very difficult to shield a physical system against noise, be it from the environment or the manipulations made over the state. Then it is natural to ask whether it is possible to perform an operation that is the inverse of dillution, i.e., some *entanglement distillation* protocol which would extract a finite number of singlet states by the use of LOCC and the consumptiom of a finite number of copies of the entangled state that we have available. Then, producing a suitable number of singlet states, one could apply recursively some dilution protocol and hence perform any desired protocol.

The first distillation protocols were developed in [142, 143, 144, 145], showing the optimal distillation rates of special classes of states. General optimal distillation protocols are believed to be very hard to develop [9, 11]. A more simple question is whether a state is distillable to a maximally entangled state. In the case of two qubits, the answer is affirmative [146]. For higher dimensions, however, the correspondence does not hold anymore [147], meaning that there exists states with a small amount of entanglement which do not give a single singlet state by LOCC, even if one has an infinite number of copies of such entangled state. These states are called *bound entangled* states, in analogy to the bound states of condensed matter physics. This is a very counter-intuitive phenomenon in quantum information theory and one of very hard characterization.

Some considerable simplifications can be made. The first is the following equivalence: a bipartite state ρ is distillable iff there exists an integer n and a SLOCC transformation that maps $\rho^{\otimes n}$ into a two-qubit entangled state [147]. Since all two-qubit entangled states are distillable, we obtain a second simplification:

Theorem 17 *If a state is PPT entangled, then it is bound entangled.*

Proof: Remembering the form of a generic $SLOCC$ map given in (1.80), we consider the partial transposition of the operator $\Lambda(\rho^{\otimes n})$,

$$[\Lambda(\rho^{\otimes n})]^{T_B} = \sum_k A_k \otimes (B_k)^T (\rho^{\otimes n})^{T_B} A_k^\dagger \otimes (B_k)^* \tag{3.28}$$

If ρ is PPT entangled, then $(\rho^{\otimes n})^{T_B}$ is positive semidefinite. Let us suppose that ρ is distillable. Then there should exist Λ in the form (1.80) such that the right-hand side above is a two-qubit entangled state. But for a two-qubit state, entanglement implies in a negative partial transposition, which is a contradiction with the PPT right-hand side above. Thus, a PPT entangled state must be bound entangled, QED.

Despite being inacessible by distillation protocols, bound entanglement can be activated [148]. Moreover, there are many applications of bound entanglement in quantum information protocols; some examples include: communication using zero-capacity channels [149], quantum cryptography [150], channel discrimination [151] and many protocols in general [152].

On the existence of NPT bound entanglement

Theorem 17 means that if a state is distillable then it is NPT. The converse statement, however, is not known up to this date. The existence of NPT bound entangled states is conjectured according to some evidences [153, 11]. If this conjecture is proven true, one remarkable corollary is the existence of bound entangled states ρ and σ such that their combination $\rho \otimes \sigma$ is distillable [154].

Peres conjecture

It has been shown that any PPT state does not violate the Bell-CHSH inequality [155], which is an upper bound on any LHVT inequality [61]. This motivated Peres to conjecture that any PPT state admits a description by a LHVT [156]. For the multipartite case this conjecture proved to be false [157], but for a bipartite system the conjecture is still open.

Smolin state

An elegant example of bound entangled state in finite dimensions was construct by Smolin [158]. It is a state in a four-partite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \mathcal{H}_D$ defined by

$$\rho_{abcd} = \frac{1}{4}\sum_{i=1}^{4} |\Psi^i_{AB}\rangle\langle\Psi^i_{AB}| \otimes |\Psi^i_{CD}\rangle\langle\Psi^i_{CD}| \tag{3.29}$$

where $|\Psi^i\rangle$ refers to one of the Bell states. The construction is such that no two parties - in separate laboratories - can distill pure entanglement, even with the help of the other parties. The only way to obtain a Bell state is when two parties come together in the same laboratory and perform nonlocal projections into Bell states. Since this strategy ends with an entangled state, (3.29) must be entangled. But if the four scientists are in different labs - meaning that only four-partite separable operations are allowed - the state is bound entangled.

Smolin state is connected to many interesting protocols, such as superactivation [159] and remote quantum information concentration [160]. For the purposes of this thesis, Smolin states are one of the few examples of bound entangled states implemented in laboratory, as we will see shortly.

3.4.1 Bound entanglement in continuous variables

Infinite dimensional systems make the problem of finding bound entangled states even harder. It was proven in [161] that bound entangled states are nowhere dense in the set of all states. Hence, even if one finds an example of bound entangled state in this regime, the odds are that any small fluctuation will bring it to the set of distillable states.

One should also define what is meant by a trully infinite-dimensional bound entangled state. One manner of trivially generating an infinite dimensional bound entangled state is by taking, for example, any $3 \otimes 3$ bound entangled state σ and then extending it to infinte dimensions. To perform this, it is a matter of finding a decomposition of the infinite-dimensional Hilbert space $\mathcal{H}$ into direct sums of $3 \otimes 3$ subspaces $\mathcal{H}_n$, i.e., $\mathcal{H} = \bigoplus_{i=0}^{\infty} \mathcal{H}_n$ so that we define the state

$$\sigma' = \bigoplus_{i=0}^{\infty} p_n \sigma_n \tag{3.30}$$

where $\{p_n\}$ is a probability distribution and σ_n means the operator σ supported on $\mathcal{H}_n$. Then the resulting state σ' is bound entangled, but this has obviously nothing to do with continuous variables. A consistent definition of continuous variable bound entanglement was found in [115]:

Definition 10 *A state represents a generic continuous variable bound entangled state if it has infinite Schmidt rank.*

With these remarks in mind, the authors proceed to construct a first example of bound entangled state in continuous variables, which we briefly consider in what follows.

Horodecki-Lewenstein state

In [115], the first continuous variables example of bipartite bound entanglement was presented. Some initial definitions are[10]:

$$|\Psi\rangle = \sum_{n=0}^{\infty} a_n |n,n\rangle; \quad ||\Psi||^2 = \sum_{n=0}^{\infty} |a_n|^2 = q < \infty; \tag{3.31}$$

$$|\Psi_{mn}\rangle = c_m a_n |n,m\rangle + (c_m)^{-1} a_m |m,n\rangle \tag{3.32}$$

The so-called Horodecki-Lewenstein state is then given by

$$\rho_{HL} = \frac{1}{A}\left(|\Psi\rangle\langle\Psi| + \sum_{n=0}^{\infty} \sum_{m>n}^{\infty} |\Psi_{mn}\rangle\langle\Psi_{mn}| \right) \tag{3.33}$$

where $A = ||\Psi||^2 + \sum_{n=0}^{\infty} \sum_{m>n}^{\infty} ||\Psi_{mn}||^2$ is a normalization factor. Since $\rho_{HL} = \rho_{HL}^{T_B}$, the state is trivially PPT. The detection of entanglement is achieved by the Range Criterion. It is important to notice that the authors did not concluded that the state has infinite Schimidt rank, so the question of generic continuous variable bound entanglement is still open. There is also not a simple way of implementing the state in practice, despite the proposal described in the reference.

[10] In the reference [115], the authors begin all sums in 1, which is apparently a typographical mistake, or at least a not usual convention. We will begin the sums in 0, but this does not affect the results.

Gaussian states

In quantum optics, Gaussian states and operations are easilly implementable in a laboratory. Their mathematical description is also very simple and elegant. The distillability of this class of states is completely characterized in the literature. Gaussian operations alone are not able to distill any entanglement [162, 163]. In fact, it is proved in [116] the distillability of all Gaussian states of the form $1 \otimes N$, i.e., a bipartite Gaussian state of many modes where the bipartition is between one mode and N modes of the field. Hence, there are no bimodal Gaussian bound entangled states. In the same reference, however, the authors construct an example of a $2 \otimes 2$ Gaussian state that is bound entangled. Thus, a multimodal Gaussian state can possess undistillable entanglement. To generate a two-mode continuous variable bound entangled state one necessarily has to move it out from the Gaussian class of states, by implementing some non-Gaussian operation over a Gaussian state (deGaussification). This is the route we follow in order to construct our example of bipartite bound entangled state in continuous variables, which we explain now.

3.4.2 A new class of bound entanglement

In this part, we present the theoretical construction of a new class of bipartite bound entangled state in continuous variables[11]. This construction will be based on realistic procedures in quantum optical setups, enabling an experimental proposal which is explained in the final section of this chapter. Let us consider first a one-mode state that is diagonal in Fock representation:

$$\rho_i = \sum_{n=0}^{\infty} p_n |n\rangle\langle n| \tag{3.34}$$

The photocounting distribution $\{p_n\}$ determines all the properties of the state; in particular, there are elegant methods to fully characterize the P-representability of ρ_i [113]. If state (3.34) is incident on a $50:50$ ($\theta = \pi/4$) BS (3.11), we obtain

$$\rho = U(\pi/4)\,(\rho_i \otimes |0\rangle\langle 0|)\,U^\dagger(\pi/4) = \sum_{n=0}^{\infty} p_n |\psi_{n,0}\rangle\langle\psi_{n,0}|, \tag{3.35}$$

where

$$|\psi_{n,0}\rangle = U(\pi/4)|n,0\rangle = \frac{1}{2^{n/2}} \sum_{k=0}^{n} \binom{n}{k}^{1/2} |k, n-k\rangle, \tag{3.36}$$

[11]This work [164] was developed in collaboration with J. Sperling and W. Vogel, from the University of Rostock.

In terms of Fock basis, the state (3.35) reads

$$\rho = \sum_{n=0}^{\infty} p_n \sum_{k,k'=0}^{n} c_{k,k'}^{(n)} |k, n-k\rangle\langle k', n-k'|, \tag{3.37}$$

where we introduced the symbols $c_{k,k'}^{(n)} = \frac{1}{2^k}\sqrt{\binom{n}{k}\binom{n}{k'}}$. We proceed now in order to find the structure of the partial transposition of the density matrix ρ, which is obtained performing the operation of transposition in only one of the subsystems. From expression (3.35) and using permutation invariance,

$$\rho = \sum_{n=0}^{\infty} p_n \sum_{k,k'=0}^{n} c_{k,k'}^{(n)} |k, n-k\rangle\langle n-k', k'|, \tag{3.38}$$

hence the partial transposed matrix of the second mode in Fock basis is given by

$$\rho^{T_B} = \sum_{n=0}^{\infty} p_n \sum_{k,k'=0}^{n} c_{k,k'}^{(n)} |k, k'\rangle\langle n-k', n-k|. \tag{3.39}$$

An arbitrary element of this matrix is

$$\langle a, b|\rho^{T_B}|c, d\rangle = \sum_{n} p_n \sum_{k,k'=0}^{n} c_{k,k'}^{(n)} \delta_{a,k}\delta_{b,k'}\delta_{c,n-k'}\delta_{d,n-k},$$

and we have then $\langle a, b|\rho^{T_B}|c, d\rangle = 0$ unless $a + d = c + b = n$, or, equivalently, $a - b = c - d$. Taking this rule into account, we choose a special ordering of the basis of the Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ so that the matrix ρ^{T_B} has a special block structure in this ordering. Let us first define the following sets:

$$\mathcal{B}_0 = \{|j, j\rangle\}_{j=0}^{\infty}, \tag{3.40}$$

$$\mathcal{B}_{+i} = \{|i + k, k\rangle\}_{k=1}^{\infty}, \tag{3.41}$$

$$\mathcal{B}_{-i} = \{|k, i + k\rangle\}_{k=1}^{\infty}. \tag{3.42}$$

The notation should be clear: the elements in the set $\mathcal{B}_0$ are vectors $|ab\rangle$ which fulfill $a - b = 0$, while elements in set $\mathcal{B}_{\pm i}$ are those which respect $a - b = \pm i$. The union of these sets is precisely the basis of the total Hilbert space $\mathcal{H}$, but now in a different ordering, i.e., we are ordering vectors $|ab\rangle$ according to their difference $a - b$. If we take as our ordered basis $\mathcal{B} = \bigcup_i \mathcal{B}_i$, the partially transposed matrix will show the block structure

$$\rho^{T_B} = \left(\begin{array}{c|c|c|c|c} \ddots & & & & \\ \hline & M_{-1} & & & \\ \hline & & M_0 & & \\ \hline & & & M_{+1} & \\ \hline & & & & \ddots \end{array}\right), \tag{3.43}$$

and we write

$$\rho^{T_B} = \bigoplus_{i=-\infty}^{\infty} M_i, \tag{3.44}$$

with each block M_i having the matricial representation

$$M_{\pm i} \overset{\mathcal{B}_{\pm i}}{\equiv} \begin{pmatrix} p_i c_{i,0}^{(i)} & p_{i+1} c_{i,0}^{(i+1)} & p_{i+2} c_{i,0}^{(i+2)} & \cdots \\ p_{i+1} c_{i+1,1}^{(i+1)} & p_{i+2} c_{i+1,1}^{(i+2)} & p_{i+3} c_{i+1,1}^{(i+3)} & \cdots \\ p_{i+2} c_{i+2,2}^{(i+2)} & p_{i+3} c_{i+2,2}^{(i+3)} & p_{i+4} c_{i+2,2}^{(i+4)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

where the notation $X \overset{\mathcal{C}}{=}$ means the matricial representation of X in the basis $\mathcal{C}$. Thus, the state ρ will be PPT iff all the blocks M_i are positive semidefinite for all values $i \in Z$.

To show the direct-sum decomposition in another way, we define $\mathcal{H}_i = Span\{\mathcal{B}_i\}$ ($Span\{.\}$ amounts to the linear span of $\{.\}$) and we have the direct-sum decomposition of the total Hilbert space as

$$\mathcal{H} = \bigoplus_{i=\infty}^{\infty} \mathcal{H}_i. \tag{3.45}$$

The subspaces $\mathcal{H}_i$ are invariant under the action of the operator ρ^{T_B}, i.e., this operator does not send vectors from $\mathcal{H}_i$ to a different $\mathcal{H}_j$. So, the operator ρ^{T_B} should decompose as a direct-sum [165].

Each block in (3.45) can be decomposed as a Hadamard product $M_i = A_i \circ B_i$, where

$$A_i = \begin{pmatrix} p_{|i|} & p_{|i|+1} & p_{|i|+2} & \cdots \\ p_{|i|+1} & p_{|i|+2} & p_{|i|+3} & \cdots \\ p_{|i|+2} & p_{|i|+3} & p_{|i|+4} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{3.46}$$

$$B_i = \begin{pmatrix} c_{i,0}^{(i)} & c_{i,0}^{(i+1)} & c_{i,0}^{(i+2)} & \cdots \\ c_{i+1,1}^{(i+1)} & c_{i+1,1}^{(i+2)} & c_{i+1,1}^{(i+3)} & \cdots \\ c_{i+2,2}^{(i+2)} & c_{i+2,2}^{(i+3)} & c_{i+2,2}^{(i+4)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{3.47}$$

We need the following theorem, known as the *Schur Product Theorem* [18]:

Theorem 18 *The Hadamard product of two positive semidefinite matrices is a positive semidefinite matrix.*

We prove now the following lemma:

Lemma 4 *The matrices B_j are positive definite, for all $j \in Z$.*

Proof: First, starting from the definition $c_{i,j}^{(k)} = \frac{1}{2^k}\sqrt{\binom{k}{i}\binom{k}{j}} = \frac{k!}{2^k}\sqrt{\frac{1}{i!j!(k-i)!(k-j)!}}$, we express an arbitrary B_j as a Hadamard product of six matrices:

$$B_j = C_j \circ D_j \circ E_j \circ E_j^{\dagger} \circ F_j \circ F_j^{\dagger}, \tag{3.48}$$

with

$$C_j = \begin{pmatrix} j! & (j+1)! & (j+2)! & \dots \\ (j+1)! & (j+2)! & (j+3)! & \dots \\ (j+2)! & (j+3)! & (j+4)! & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

$$D_j = \begin{pmatrix} 1/2^j & 1/2^{j+1} & 1/2^{j+2} & \dots \\ 1/2^{j+1} & 1/2^{j+2} & 1/2^{j+3} & \dots \\ 1/2^{j+2} & 1/2^{j+3} & 1/2^{j+4} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

$$E_j = \begin{pmatrix} 1/\sqrt{0!} & 1/\sqrt{0!} & 1/\sqrt{0!} & \dots \\ 1/\sqrt{1!} & 1/\sqrt{1!} & 1/\sqrt{1!} & \dots \\ 1/\sqrt{2!} & 1/\sqrt{2!} & 1/\sqrt{2!} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

$$F_j = \begin{pmatrix} 1/\sqrt{j!} & 1/\sqrt{j!} & 1/\sqrt{j!} & \dots \\ 1/\sqrt{(j+1)!} & 1/\sqrt{(j+1)!} & 1/\sqrt{(j+1)!} & \dots \\ 1/\sqrt{(j+2)!} & 1/\sqrt{(j+2)!} & 1/\sqrt{(j+2)!} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

The matrices D_j, E_j and F_j are rank-1 matrices, so are obviously positive. The Hankel matrix C_0 is positive definite, since its leading principal minors of order k have determinant $\Pi_{i=0}^{k}(i!)^2$. A similar argument holds for an arbitrary C_j and thus they are all positive definite. Another way to prove this is observing that the following sequence satisfies the Stieltjes moment problem[12] [166]:

$$f_n = n! = \int_0^{\infty} x^n e^{-x} dx, \quad n = 0, 1, 2, \dots \tag{3.49}$$

[12]This means here that the Hankel operator whose elements are the sequence satisfying the moment problem is a positive definite operator.

So, C_0 is positive definite. Now, we see that

$$\begin{aligned}
g_0 &= j! = \int_0^\infty x^0(x^j e^{-x})dx, && (3.50)\\
g_1 &= (j+1)! = \int_0^\infty x^1(x^j e^{-x})dx, && (3.51)\\
g_2 &= (j+2)! = \int_0^\infty x^2(x^j e^{-x})dx, && (3.52)\\
&\vdots && (3.53)
\end{aligned}$$

defines a sequence that also satisfies the Stieltjes moment problem. From Theorem 1, the Hadamard product of positive-semidefinite matrices is a positive-semidefinite matrix. Also, the Hadamard product of a positive-definite matrix - C_j in our case - with rank-1 matrices - D_j, E_j and F_j - is positive-definite[13]. So B_j is a positive-definite matrix, QED.

With these preliminaries results, we can prove the following proposition, which relates the photocounting distribution of the input state ρ_i to the PPT property of the output state (3.35).

Proposition 1 *State (3.35) is PPT if the following infinite-dimensional Hankel matrix* [14]

$$A_0 = \begin{pmatrix} p_0 & p_1 & p_2 & \cdots \\ p_1 & p_2 & p_3 & \cdots \\ p_2 & p_3 & p_4 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{3.54}$$

is positive semidefinite.

Proof: Since all B_i are positive definite, to have all M_i positive semidefinite we must have all A_i positive semidefinite. But A_0 positive semidefinite implies, by Sylvester's Criterion, that all other A_i are positive semidefinite, since they are principal submatrices of A_0. So, all $M_i = A_i \circ B_i$ are positive semidefinite if A_0 is positive semidefinite

[13]The Hadamard product of a positive-definite matrix with the rank-1 matrices of the form D_j, E_j and F_j does not affect the leading principal minors' positivity: multipliyng rows of a square matrix by a positive constant do not change the sign of the determinant of this matrix. This implies that positive-definiteness is preserved.

[14]A Hankel matrix is a matrix whose coefficients depend on the sum of rows and columms, i.e., $h_{ij} = h_{i+j}$, having thus constant elements along skew-diagonals.

and by the block structure of ρ the state is PPT if A_0 is positive semidefinite, QED.

Thus the positivity under partial transposition can be checked by a hierarchical sequence of photocounting probabilities matrices. Indeed, a similar connection is already present in reference [113] with regard to the Stieltjes moment problem, in terms of nonclassicality exhibited by states Negative under Partial Transposition (NPT). An advantage of our approach is the direct-sum structure in Eq. (3.44), which allows us to handle the construction of PPT states in a simple way. Similar direct-sum decompositions of the partially transposed density matrix can be found in [132, 168] and bring a great deal of simplification when dealing with PPT bound entanglement.

The state (3.35) alone cannot generate PPT-bound entangled states, as shown in reference [113]. We thus consider a more general class of states, given by

$$\rho' = \lambda\rho + (1-\lambda)|\Omega\rangle\langle\Omega|, \tag{3.55}$$

corresponding to the mixture of state ρ in (3.35) with the state

$$|\Omega\rangle = (1-|\omega|^2)^{1/4}\sum_{k=0}^{\infty}\sqrt{\frac{\Gamma(n+1/2)}{n!\sqrt{\pi}}}\omega^k|\phi_{2k,0}\rangle, \tag{3.56}$$

State (3.56) is generated by passing a one-mode squeezed vacuum state,

$$|0_{sq}\rangle = (1-|\omega|^2)^{1/4}\sum_{k=0}^{\infty}\sqrt{\frac{\Gamma(n+1/2)}{n!\sqrt{\pi}}}\omega^k|2k\rangle, \tag{3.57}$$

generated in an optical parametric oscillator, through a second BS. Here $\omega = (\xi/|\xi|)\tanh(|\xi|/2)$ is the squeezing parameter and thus $0 < |\omega| < 1$. We impose for the second BS that the parameter θ in (3.11) satisfy $\theta \neq \pi/4$, i.e, the second BS is not a $50:50$ beam-splitter. For simplicity, we take $0 < \theta < \pi/4$. Thus we have

$$|\Omega\rangle = U(\theta)|0_{sq}\rangle, \tag{3.58}$$

and writing $|\phi_{n,0}\rangle = U(\theta)|n,0\rangle$, we arrive at expression (3.56), with

$$|\phi_{2k,0}\rangle = \sum_{l=0}^{2k}\binom{2k}{l}^{1/2}(\cos\theta)^l(\sin\theta)^{2k-l}|l,2k-l\rangle. \tag{3.59}$$

We will impose that the input state (3.34) be given by a state of the form,

$$\rho_i = \sum_{n=0}^{\infty}\frac{1}{\bar{n}+1}\left(\frac{\bar{n}}{\bar{n}+1}\right)^n|n+1\rangle\langle n+1|, \tag{3.60}$$

where $\bar{n}$ is the mean thermal photon number. This class of states is known as a *shifted-thermal state* and will be explained in further sections. The shifted thermal state allows the state (3.55) to have genuine bound entanglement as we discuss later on.

Observation 4 *State (3.55) is entangled for any* $0 < |\omega| < 1$.

Proof: We will use the Range Criterion of separability (Theorem 14). A violation of at least one of the conditions of this criterion implies entanglement, thus we prove that the range of ρ' in (3.55) does not contain a single product vector. The range of ρ' is spanned by $\{|\psi_{n,0}\rangle\}$ - with $n = 0, 1, \dots, \infty$ - and $|\Omega\rangle$ as given in Eqs. (3.36) and (3.56), respectively. We show now that assuming a product vector in the range of ρ' leads to a contradiction.

Thus, let us assume that there exist complex numbers m_k, $k = 0, 1, 2, \dots$ such that

$$m_0|\Omega\rangle + \sum_{k=1}^{\infty} m_k|\psi_{k,0}\rangle = |v_1\rangle \otimes |v_2\rangle \tag{3.61}$$

where

$$|v_1\rangle = \sum_{k=0}^{\infty} \alpha_k|k\rangle, |v_2\rangle = \sum_{k'=0}^{\infty} \beta_{k'}|k'\rangle. \tag{3.62}$$

Let us write explicitly some important terms in left-hand side of (3.61):

$$\begin{aligned}
& m_0|0,0\rangle + m_1\left(|0,1\rangle + |1,0\rangle\right) + \left((\omega/\sqrt{2})m_0\cos^2\theta + m_2\right)|0,2\rangle \\
+ \quad & \left((\omega/\sqrt{2})m_0\sin\theta\cos\theta + \sqrt{2}m_2\right)|1,1\rangle + \left((\omega/\sqrt{2})m_0\sin^2\theta + m_2\right)|2,0\rangle \\
+ \quad & m_3\left(|0,3\rangle + \sqrt{3}|1,2\rangle + \sqrt{3}|2,1\rangle + |3,0\rangle\right) \\
+ \quad & \left(m_0\omega^2(3/8)\cos\theta\sin^3\theta + m_4\sqrt{4}\right)|1,3\rangle + \left(m_0\omega^2(3/8)\cos^3\theta\sin\theta + m_4\sqrt{4}\right)|3,1\rangle \\
+ \quad & \dots
\end{aligned}$$

We disregard normalization factors, since one can always incorporate these factors in the values m_i. The first terms in the right-hand side of (3.61) are

$$\begin{aligned}
& \alpha_0\beta_0|0,0\rangle + \alpha_0\beta_1|0,1\rangle + \alpha_1\beta_0|1,0\rangle + \alpha_0\beta_2|0,2\rangle \\
+ \quad & \alpha_1\beta_1|1,1\rangle + \alpha_2\beta_0|2,0\rangle \\
+ \quad & \alpha_0\beta_3|0,3\rangle + \alpha_1\beta_2|1,2\rangle + \alpha_2\beta_1|2,1\rangle + \alpha_3\beta_0|3,0\rangle \\
+ \quad & \alpha_1\beta_3|1,3\rangle + \alpha_3\beta_1|3,1\rangle \\
+ \quad & \dots
\end{aligned}$$

Let us first assume $m_0 = 0$, this implies $\alpha_0\beta_0 = 0$, by the linear independence of the set $\{|i,j\rangle\}$ - with $i,j = 0,1,\ldots,\infty$. Hence either $\alpha_0 = 0$ or $\beta_0 = 0$; it is straightforward that either case would imply $m_i = 0$ for all i, clearly being a contradiction. Let us then consider the case $m_0 \neq 0$. Without loss of generality, we assume $\alpha_0 = \beta_0 = 1$; from expression (3.61), one gets $m_0 = 1$ and since $\{|\psi_{n,0}\rangle\}$ is permutationally invariant, for all $n = 0,1,\ldots,\infty$, we have for the first odd terms $m_1 = \alpha_1 = \beta_1$, and $m_3 = \alpha_3 = \beta_3$. So $\alpha_1\beta_3 = \alpha_3\beta_1$. However, we have for the corresponding terms $\alpha_1\beta_3 = m_0\omega^2(3/8)\cos\theta\sin^3\theta + m_4\sqrt{4}$, and $\alpha_3\beta_1 = m_0\omega^2(3/8)\cos^3\theta\sin\theta + m_4\sqrt{4}$. Since $\theta \neq \pi/4$, we conclude that $\alpha_3\beta_1 \neq \alpha_1\beta_3$, a contradiction [15]. Thus, there is no product vector in the range of ρ', implying Observation 1 is true, QED.

The idea to obtain a PPT (3.55) is that the only block (3.44) for the shifted-thermal state that is negative under partial transposition is the block M_0, due to $p_0 = 0$. Hence, with a suitable small squeezing parameter ω, the vacuum amplitude of the squeezed state, i.e $|\langle 00|\Omega_{sq}\rangle|^2 = \sqrt{1-|\omega|^2}$ will be suitably big in such a way to replace the null vacuum amplitude of ρ, making the mixture ρ' positive under partial transposition. The other terms are $O(|\omega|)$, being as small as one desires, representing a small perturbation under control. We obtain thus:

Observation 5 *There exists states (3.55) which are PPT. By Observation 1 these states are bound entangled.*

Proof: For simplicity, we will construct a example of a PPT (3.55) with $\lambda = 1/2$ and ρ being the output of (3.84) with $\bar{n} = 1$. Thus, the state we are considering is

$$\rho' = \frac{1}{2}\left(\rho + |\Omega\rangle\langle\Omega|\right) \tag{3.63}$$

with

$$\rho = \sum_{n=1}^{\infty}\left(\frac{1}{2}\right)^n |\psi_{n0}\rangle\langle\psi_{n0}| \tag{3.64}$$

We first observe that any shifted thermal state ρ generated by (3.84) is locally equivalent to (3.64) above. Define the following invertible operation:

$$T|n\rangle = (\bar{n}+1)^{1/2}\left(\frac{\bar{n}+1}{2\bar{n}}\right)^{n/2}|n\rangle \tag{3.65}$$

[15] For $\theta = \pi/4$ there is not a contradiction and state (3.55) would be permutationally symmetric in the sense of [114]. In this reference, there is a method to construct entanglement witnesses to detect entanglement of permutationally symmetric states. We will let the separability of this special case as an open (and interesting) question.

Then we have that $T \otimes T\rho T^\dagger \otimes T^\dagger$ is equal to the matrix (3.64). Local invertible operations do not affect positivity of the partial transposed matrix, thus this special case is broad in this sense (for the case of $\lambda = 1/2$).

We know that (3.64) is NPT, since $p_0 = 0$, implying that ρ_i is nonclassical and thus NPT, by the criterion of [113]. Also, from (3.44), we know that

$$\rho^{T_B} = \bigoplus_{i=-\infty}^{\infty} M_i \tag{3.66}$$

where $M_i = A_i \circ B_i$. For $i \neq 0$, the blocks, M_i are all positive definite, since the corresponding matrices A_i are positive definite. When we consider the new partially transposed matrix for (3.63), we have

$$\rho'^{T_B} = (1/2)(\rho^{T_B} + |\Omega\rangle\langle\Omega|^{T_B}). \tag{3.67}$$

We will now consider that $|\omega|$ is sufficiently small that we can neglect terms $O(|\omega^2|)$; we will discuss more on this point in what follows. Thus, in this approximation we can say that effectively we have $|\Omega\rangle\langle\Omega|^{T_B} \approx (\sqrt{1-|\omega|^2})(|00\rangle\langle 00| + \omega|\phi_{20}\rangle\langle 00| + \omega|00\rangle\langle\phi_{20}|)$. We can rewrite Eq. (3.67) as

$$\rho'^{T_B} = (1/2)\left[\left(\bigoplus_{i=-\infty}^{\infty} M_i'\right) + P\right], \tag{3.68}$$

where $M_i' = M_i$, for $i \neq 0$ and $M_0' = M_0 + \sqrt{1-|\omega|^2}|00\rangle\langle 00|$, while $P = \omega(|\phi_{20}\rangle\langle 00| + |00\rangle\langle\phi_{20}|)^{T_B}$ represents a perturbation with magnitude totally dependent on the value of $|\omega|$.

It is straightforward that for values $\sqrt{1-|\omega|^2} > 1/2$, which means $|\omega| < \sqrt{3/4}$, the block M_0' becomes positive-definite. We must know how small $|\omega|$ must be so that ρ'^{T_B} remains positive.

Remark: *Since the eigenvalues of a matrix are continuous functions of its elements, we could already stop the demonstration at this point: slight variations of ω would not affect the eigenvalues of the positive blocks M_i' significantly and consequently its positivity. However, the constructive demonstration given here has the advantage of giving an estimate on the order of magnitude of the value ω, which is relevant experimentally.*

We need the following theorem (Theorem 6.1.1 from [18]), known as the Gerschgorin Disc Theorem:

Theorem 19 *Given a $n \times n$ square matrix $M = [m_{ij}]$, let*

$$R_i(M) \equiv \sum_{j=0, j\neq i}^{n-1} |m_{ij}|, \quad i = 0, 1, \ldots, n-1, \tag{3.69}$$

denote the deleted absolute row sums of M. Then all the eigenvalues of M are located in the union of n discs

$$\bigcup_{i=0}^{n-1}\{z \in \mathcal{C} : |z - a_{ii}| \leq R_i(M)\} \equiv G(M). \tag{3.70}$$

Furthermore, if a union of k of these n discs form a connected region that is disjoint from all the remaining $n-k$ discs, then there are precisely k eigenvalues of M in this region.

The region $G(M)$ is called the Gerschgorin region of M and the individual discs in $G(M)$ are called Gerschgorin discs; the boundaries of these discs are called the Gerschgorin circles. A similar result holds for the collum-sums (Corollary 6.1.3 from [18]), but since we are dealing with Hermitean matrices it will not affect the results. We need also the following refinement (Corollary 6.1.6 from [18]):

Corollary 1 *Let $D = diag\{d_0, d_1, \ldots\}$, with d_i positive real numbers for all $i = 0, 1, \ldots$. Then all eigenvalues of M lie in the region*

$$\bigcup_{i=0}^{n-1}\{z \in \mathcal{C} : |z - a_{ii}| \leq \frac{1}{d_i}\sum_{j=0,j\neq i}^{n-1} d_j|m_{ij}|\} \equiv G(D^{-1}MD).$$

Moreover, the spectrum of M is precisely[16] *the set $\bigcap_D G(D^{-1}MD)$.*

Since the blocks M_i' are all positive-definite, there exists a set of d_is above which will bring all Gerschgorin disks to the positive segment of the real line. Also, there is a continuous of such d_i's and we conclude then that a slight change in the row sums R_i - which are constituted by the off-diagonal elements of the matrix - will not change the eigenvalues of a matrix, since this would correspond to a negligible deformation of the corresponding Gerschgorin region. Let us see how this applies to example (3.63).

[16]We give a simple example of this method for the matrix

$$M = \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix}. \tag{3.71}$$

The Gerschgorin disks of Theorem 19 are given by $|z-1| \leq 1$ and $|z-2| \leq 0$ which gives $0 \leq z \leq 2$ and $z = 2$. The Gerschgorin region is then $0 \leq z \leq 2$ and we cannot say very much about the eigenvalues. Now, applying the refinement given by Corollary 1, we arrive at equations $1-(d_2/d_1) \leq z \leq 1+(d_2/d_1)$ and $z = 2$, which are disjoint intervals for any $d_2 < d_1$. Hence, one sure eigenvalue is 2, while the other is known to be around the value 1.

The perturbation matrix P affects only the first row and collum of each M_0', $M_{\pm 1}'$ and $M_{\pm 2}'$. For the first lines of these blocks we have

$$|z_0 - \sqrt{1-\omega^2}| \leq 2\omega + R_0 \tag{3.72}$$

$$|z_1 - \frac{p_1}{2}| \leq \omega + R_1 \tag{3.73}$$

$$|z_2 - \frac{p_2}{4}| \leq \omega + R_2 \tag{3.74}$$

By putting the sole value ω, instead of the actual terms $\omega\cos^2(\theta)$, $\omega\sin^2(\theta)$ and $\omega\sin(\theta)\cos^2(\theta)$, we are doing an overstimation of the perturbation. By the equations above, if $|\omega| << p_2/4 < p_1/2 < \sqrt{1-|\omega|^2}$, we will have that ρ'^{T_B} will remain positive, since the associated Gerschgorin regions will be effectivelly unaffected. The value $p_2/4 = 1/16$ has a order of magnitude of 10^{-2}; thus we will impose for $|\omega|$ a conservative upeer bound of 10^{-3}. We can now justify the neglecting of terms $O(\omega^2)$: their rate of decrease is much faster than the rate of decrease of diagonal elements; also, we have not considered terms $\sin^k(\theta)\cos^{1-k}(\theta)$, which would make this rate even faster, QED.

Although in practice, for continuous variable's regime it is analytically and numerically hard to determine exactly [17] the spectrum of ρ', it is possible to obtain upper bounds for the values of $|\omega|$, which guarantee a positive partial transposition. For the example considered, a conservative upper bound of $|\omega| \leq 10^{-3}$ has proved to be sufficient, allowing the generation of a bound entangled state in continuous variables. It will remain an open question whether we have found or not a *generic* continuous variable bipartite bound entangled state, i.e., a bound entangled state with infinite Schmidt rank [115]. With this in mind, we now proceed to explain how to actually implement the class of states (3.55).

[17] This comes from two reasons. First, the underlying Hankel structure of the partially transposed matrix imposes a numerical ill-conditioning (see [167]). The second and more severe reason is that there are no general results about the eigendecomposition of a Hadamard product of two matrices. So, even if one finds a good Hankel matrix structure, the various Hadamard products can spoil the whole process.

3.5 Experimental implementation of bound entanglement

We present here the main experiments that implement bound entanglement using quantum optical setups. An important experiment involving ion-traps which is not reviewed here is given in [174]. We recently became aware of an experiment implementing a finite-dimensional example of bound entanglement in quantum optics [175], using the separability criterion [49], which uses relations of complementarity similar to the relations developed by Luis [50]. None of the experiments implement a genuinely bipartite bound entangled state in continuous variables and hence our proposal, described in the final section of this chapter, is both a theoretical and practical improvement over previous results.

3.5.1 Previous work

The first experiment that attempted the preparation of a bound entangled state was performed by Amselem and Bourennane [176]. The authors pursuited the implementation of the Smolin state (3.29) in a very clever way. Let us write again the expression of the state, for clarity:

$$\rho_{abcd} = \frac{1}{4}\sum_{i=1}^{4} |\Psi^i_{AB}\rangle\langle\Psi^i_{AB}| \otimes |\Psi^i_{CD}\rangle\langle\Psi^i_{CD}| \tag{3.75}$$

Let us also make explicit the labelling and how to obtain each state by local rotations:

$$|\Psi^1\rangle \equiv |\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle); \tag{3.76}$$

$$|\Psi^2\rangle \equiv |\psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) = (\sigma_z \otimes I)|\psi^-\rangle; \tag{3.77}$$

$$|\Psi^3\rangle \equiv |\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) = (I \otimes \sigma_x)|\psi^-\rangle; \tag{3.78}$$

$$|\Psi^4\rangle \equiv |\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = (\sigma_z \otimes \sigma_x)|\psi^-\rangle; \tag{3.79}$$

We see then that if one has a source of singlets $|\psi^-\rangle$, then all other Bell-states in the decomposition of the Smolin state can be obtained performing local Pauli matrices rotations. This is what is done in the experiment, as is shown in the scheme of Fig. 3.1.

Despite indeed generating the Smolin state with a high fidelity, the experimental data did not support a PPT state, as pointed out by Lavoie *et. al.* in [177]. The

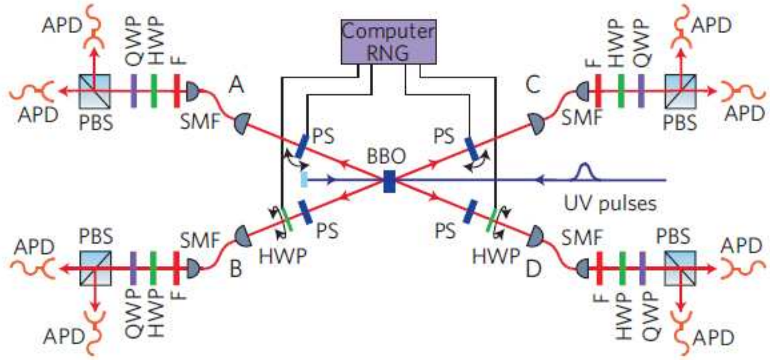

Figure 3.1: A UV pulse incides on a BBO-crystal and then is reflected in the opposite direction onto the same crystal, producing a state $|\psi^-_{AB}\rangle\langle\psi^-_{AB}| \otimes |\psi^-_{CD}\rangle\langle\psi^-_{CD}|$ by spontaneous parametric down conversion. With probability 1/4 controlled by a Random Number Generator (RNG), local Pauli gates are applied, generating the desired terms in (3.29) through the relations (3.79). The beams proceed to Polarizing Beam-Splitters (PBS) and Avalanche Photo-Diode (APD) detectors, in order to reconstruct the state.

minimal eigenvalue of the partial transposed matrix reported is -0.02 ± 0.02, thus the value is not surelly positive. One cannot claim that this state is PPT bound entangled.

The reason for this negative result comes from the fact that the partial transposition of the Smolin state is not a full-rank matrix. Any uncontrollable small perturabation in the experiment would produce similar results. This observation motivated the authors of reference [177] to propose a version of the Smolin state that is robust against experimental fluctuations. The idea is simple and easy to implement in laboratory, since it demands just a small modification of the seminal arrangement in [176]. One performs a statistical mixture of the Smolin state with some fraction of white noise:

$$\rho_R(p) = p\frac{I}{16} + (1-p)\rho_{abcd} \tag{3.80}$$

Then the partial transposition is full-rank and positive, but the perturbation p is small in such a way to not destruct entanglement. Lavoie *et. al.* perform then a fancier version of the experiment of Amselem and Bourennane in [178], thus reporting the first experimental implementation of bound entanglement in the literature.

The scheme of Lavoie *et. al.* was later criticized by DiGuglielmo *et. al.* in [179], on the ground that the implementation of (3.80) was conditioned[18] to the result of

[18]The authors acknowledge the experiment in [174] as the first unconditional implementation of

measurements. The authors then report an *unconditional* experimental implementation of bound entanglement, this time a continuous variable one using a $2\otimes 2$ Gaussian state, similar to the Gaussian bound entangled state of [116].

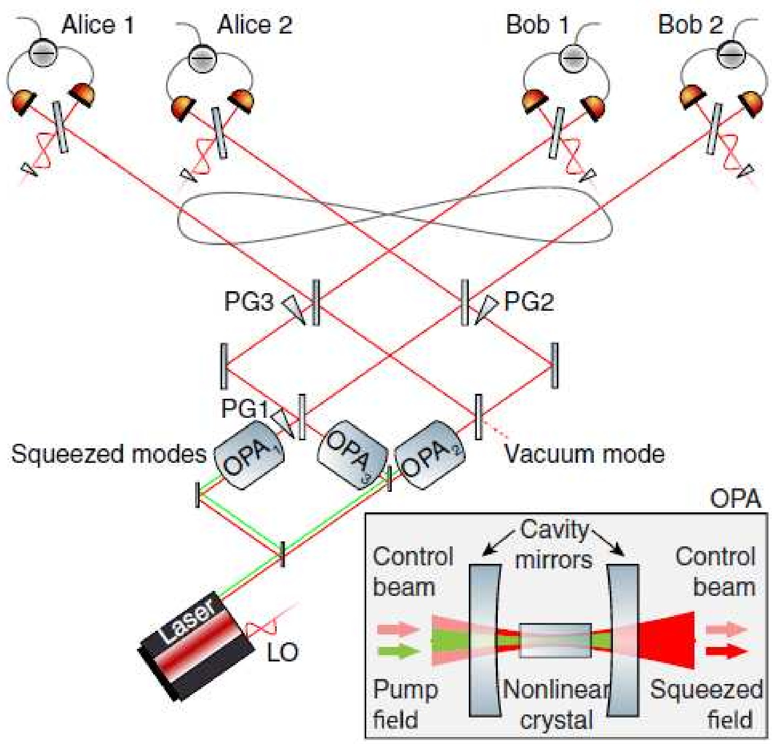

Figure 3.2: The light generated by a laser is splitted in such a way to incide in three different Optical Parametric Amplifiers (OPA), which are devices that generate squeezed light using a nonlinear crystal and cavity QED schemes. The phases are controlled by Phase Generators (PG). Notice that no conditional operation was performed. The beams proceed then to local homodyne setups for performing the tomography of the global state.

This is thus the first implementation of bound entanglement in continuous variables. The unconditional nature enables a downstream distribution of this entanglement, which is a remarkable property, with many potential applications in quantum information theory.

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bound entanglement. This experiment also implements a robust version of the Smolin state, but the state surges naturally as the result of decoherence in an ion-trap setup, without need of conditional interventions to reach the density matrix.

3.5.2 Experimental proposal

All experiments described in the previous section are designed in a multipartite setting, which is easier to design PPT entangled states. The seminal Horodecki-Lewenstein state [115], although bipartite and in continuous variables, is not easilly implementable in practice. We describe now our proposal, which overcomes all these complications and can be made unconditional afeter a calibration of the apparatus.

The procedure employed here for generating bound entanglement between two modes employs a deGaussification procedure and requires two fundamental steps - a photo-addition over a thermal state, and an incoherent mixture to a two-mode squeezed vacuum. The experimental setup is presented in Fig. 3.3.

There a V-polarized single-mode is prepared in a thermal state, $\rho_T = \sum_n p_n|n\rangle\langle n|$, with thermal distribution $\{p_n\}$, through a phase-randomization process by a rotating disk (RD)[180]. This light mode, A, is then photon-added (through a process inside the box PA to be later described), transforming $\{p_n\}$ into $\{p'_n\}$, and then mixed with a vacuum state mode, B, on the $50:50$ beam-splitter BS-1. Since an arbitrary beam-splitter action on the creation operators of two input modes is given by the global unitary operation (3.11) the output state for the $50:50$ ($\theta = \pi/4$) beam-splitter BS-1 is given by (3.35). The state (3.35) alone cannot generate PPT-bound entangled states, as shown in reference [113]. We thus have considered a more general class of states, given by (3.55)

$$\rho' = \lambda\rho + (1-\lambda)|\Omega\rangle\langle\Omega|, \tag{3.81}$$

corresponding to the mixture of state ρ in (3.35) with the state (3.56) whose preparation is depicted in Fig. 1 as we now explain. State (3.56) is generated by passing a H-polarized one-mode squeezed vacuum state,

$$|0_{sq}\rangle = (1-|\omega|^2)^{1/4}\sum_{k=0}^{\infty}\sqrt{\frac{\Gamma(n+1/2)}{n!\sqrt{\pi}}}\omega^k|2k\rangle, \tag{3.82}$$

generated in an optical parametric oscillator, through the beam-splitter BS-2. Here $\omega = (\xi/|\xi|)\tanh(|\xi|/2)$ is the squeezing parameter and thus $0 < |\omega| < 1$. We impose for BS-2 that the parameter θ in (3.11) satisfy $\theta \neq \pi/4$, i.e, not a $50:50$ beam-splitter. For simplicity, we take $0 < \theta < \pi/4$. Thus we have $|\Omega\rangle = U(\theta)|0_{sq}\rangle$ and writing $|\phi_{n,0}\rangle = U(\theta)|n,0\rangle$, we arrive at expression (3.56), with

$$|\phi_{2k,0}\rangle = \sum_{l=0}^{2k}\binom{2k}{l}^{1/2}(\cos\theta)^l(\sin\theta)^{2k-l}|l,2k-l\rangle. \tag{3.83}$$

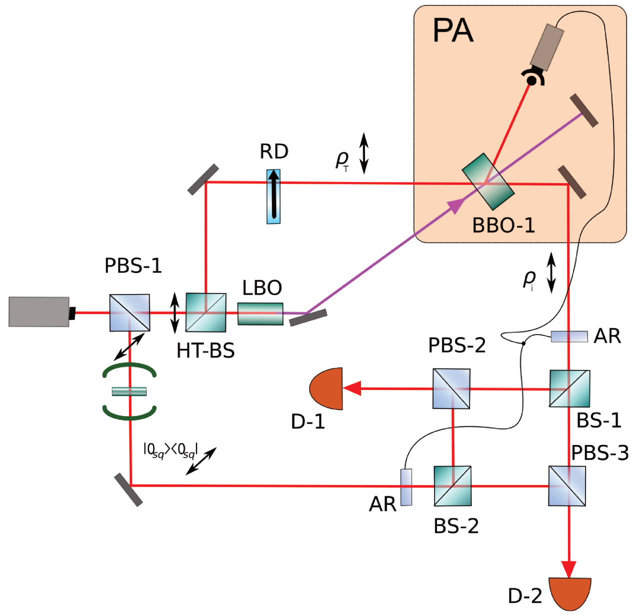

Figure 3.3: Two orthogonally polarized components of a laser beam are split in the polarizing beam splitter PBS-1. The V-polarized beam is prepared in a thermal state ρ_T through the rotating disc RD and photon-added in the process described in the box PA (see text for details) to originate state ρ_i. This mode is sent through the 50:50 beam splitter BS-1 whose output is described by Eq. (3.35). The H-polarized component of the laser beam coming out of PBS-1 is used through an optical parametric oscillator to generate a squeezed vacuum state $|0_{sq}\rangle$, which is sent through BS-2 whose output is given by Eq. (3.56). The V-polarized and H-polarized output modes of BS-1 and BS-2, respectively, are sent through PBS-2 and PBS-3 to homodyne detection processes D-1 and D-2. The active retarders (or modulators) AR allow that only one of the V or H polarizations to proceed to D-1 and D-2 conditioned to photon-addition process in PA and on external control. The resulting state coming out from reconstructions in D-1 and D-2 is given by Eq. (3.55).

Now to prepare the mixture in (3.55), the two independent preparations are recombined in the polarizing beam-splitters PBS-2 and PBS-3 and proceed for homodyne detection on D-1 and D-2. The active retarders (AR) are externally controlled by the detection of a photon in the photo-addition process plus a external control to generate the full range of λ in (3.55). Whenever this photon is detected in the idler mode generated in the parametric dow-conversion in BBO-1, indicating that a photon has been added to the signal mode, the AR allow only the V-polarized photon-added thermal component to leave to the detectors. When no photon is detected only the H-polarized two-mode squeezed vacuum is allowed to proceed to the detectors. By neglecting some of those detections, the ARs control the fraction λ of polarization of the field incident at the photodetectors for repeated experiments. The idea behind this preparation is to use the fact that the beam-splitter is a classicality- preserving device and converts a (non-)classical state into a (in)separable one. The mixing in (3.55) is thus a mixture of two nonclassical states and since the mixing parameter λ is controllable by the experimentalist through the ARs, it is possible to prepare an entangled state whose partial transposition is still positive. As we will see a crucial element here was the elimination of the vacuum component from the thermal state by the photon-addition process.

For the mixture present in Eq. (3.55) to allow a genuinely bound entangled state it is necessary to first change the Gaussian character of the V-polarized thermal state at mode A. A simple procedure to deGaussify the thermal state is the photon-addition as described in [180], which assumes that when the thermal state is fed as a signal into a parametric amplifier, the output signal state is conditionally prepared every time that a single photon is detected in the correlated idler mode. The simple assumption here is that the action of the conditioned parametric amplification is given up to first order in the coupling g between idler and signal by $[1+(ga_s^\dagger a_i^\dagger - g^* a_s a_i)]$ where $a_{s(i)}^\dagger$ are bosonic creation operators acting on the signal (idler) modes. This results in a photon-added thermal state, which although possessing the character needed (absence of the vacuum state), has failed to produce a PPT state. However if instead one is able to implement a saturated photon-addition [170] in the sense that the action of the creation and annihilation operators in the signal is replaced by $E^+ = a_s^\dagger(a_s^\dagger a_s + 1)^{-1/2}$ and $E^- = (a_s^\dagger a_s + 1)^{-1/2} a_s$ respectively, the resulting state conditioned to the detection of one photon in the idler is given by the shifted-thermal state [171],

$$\rho_i = \sum_{n=0}^{\infty} \frac{1}{\bar{n}+1}\left(\frac{\bar{n}}{\bar{n}+1}\right)^n |n+1\rangle\langle n+1|, \tag{3.84}$$

where $\bar{n}$ is the mean thermal photon number. These states were first considered by Lee in reference [171], in an analysis of the scheme depicted in [169], where laser cooling significantly changes the emission of radiation of a micromaser. The distribution (3.84) arises in [171] when the parameters of the micromaser cavity fulfill an ideal requirement. The shifting operation is also present in the related proposal of [172]. Remarkably, a scheme to prepare (3.84) deterministically has been recently proposed [173], making the unconditional preparation of (3.55) an achievable goal. The shifted thermal state allows the state (3.55) to have genuine bound entanglement as we proved in the previous section.

Summary

We have presented a procedure to unconditionally prepare bipartite bound entangled states in continuous variable's regime. The approach assumed was to deGaussify a thermal field by a photon addition process and to mix it with a squeezed vacuum state. Several minor results were developed in order to achieve this goal. Particularly the links with Hankel operator theory and the direct-sum structure of the partially transposed state allowed us to give bounds on the parameters that enable PPT bound entangled states to be produced. There are few examples of such states in continuous variables and thus the novel class (3.55) is interesting in its own, even if it were impossible to envisage a scheme to generate it experimentally. Our work shows that this is not the case and that the preparation in practice is feasible, opening new possibilities in quantum information processing protocols, as well as in the theory of quantum entanglement. We focused on thermal fields, due to their implementation simplicity in the laboratory and also due to their use in fundamental experiments as [180], but we stress that similar results could in principle be achieved with different classical photocounting distributions. Our approach was to remove the vaccum contribution of the thermal state by performing a photo-addition and then replacing it with the vaccum term of the squeezed state, which is superposed with other terms. If one is able to produce a one-mode state satisfying Proposition 1 and then could entangle its vaccum term with other convenient state, we believe it is possible to construct similar states to (3.55); this point is currently being investigated.

Summarizing, we provided a scheme for the construction of a state with the following properties:

1. It is bound entangled.
2. It is solely a bipartite state.
3. It requires continuous variables.
4. It can be generated with current experimental techniques.

Even under the highly restrictive conditions $(1-4)$, we were able to formulate a whole class of such states. Moreover, original and general methods of generation and characterization of these states are derived in our contribution.

Chapter 4

Conclusions and perspectives

In this thesis we presented many new results characterizing nonclassicality, entanglement and important relations between these two fundamental concepts. The results with major importance seem to be those concerning the mutually excludent relation between the complementarity principle and superquantum configurations. We showed that only the complementarity principle could give a consistent reason for the non-observation of phenomena beyond quantum physics. Even restrictions imposed by probability theory could leave open the possibility of superquantum configurations, as we discussed. Since the operational formulation of Luis [50] can be derived without directly resorting to the quantum formalism, it is remarkable that quantum limits are a corollary of the complementarity relations. These conclusions were natural consequences of the quasiprobability representation developed by us, a formulation in terms of MUB sets that is simple and can be extended to arbitrary prime-power dimensions. In the case of a qubit, nice relations with l_p-norms greatly simplified the constructions. For higher dimensions, an indirect method was developed, in terms of mixtures and quasi-mixtures of elements in the MUB set. We believe that similar relations in terms of l_p-norms can be obtained for higher dimensions, giving a general probabilistic formulation of the representation for arbitrary dimensions. This is being developed currently by us.

An equally relevant result was described in final sections, where the new class of entangled states (3.55) delivered bound entanglement for a certain range of the parameters involved. The theoretical constructions are not the usual ones in the literature, using infinite direct-sum decompositions of the state space, Hankel operator theory, Gerschgorin disks perturbation theorems and many other steps that are original. The physical resoning behind the proposal was to apply a deGaussification procedure over a thermal state of the radiation and then mix the resulting preparation with a two-mode vaccum-squeezed state, with squeezing degree under control. The scheme suceed in designing a class of genuine bipartite bound entangled states in continuous variables that can be generated with current experimental techniques. To be fair, we believe that today this state is not still implementable, due to present technical difficulties. However, different parts of our experimental proposal are already implemented in separated quantum optical schemes and we think that is merelly a question of updating these similar procedures and bringing them together to the same optical regime. A relevant related open problem is the development of entanglement witnesses for these states, since the experimentalist would avoid the need of quantum tomography of the state and also could detect other states. Moreover, it is possible that robust regimes of bound entanglement could be designed, an impactating possibility. This was indeed one of the starting points of this work, but the results in this direction were inconclusive; also, the proof by means of the Range Criterion was so simple and broad that we opted for letting this question to be answered by future works.

Finally, a simpler but broad result for the detection and consistent definition of nonclassicality was explained and is closely related to the task of entanglement creation. We showed an observable-based notion of nonclassicality, which can thus be employed in many different physical setups. Important simplifications due to symmetry considerations were developed, with an elegant description in terms of group coherent states. Moreover, we stressed the necessity of our approach for the understanding on how to generate entanglement with controlled operations, a topic which in some situations is ill-posed in the quasiprobability formulation. We hope that our construction can be applied to practical detection schemes, similarly to the suscessfull applications of entanglement witnesses in many different experiments.

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