Quantumness of States: From positive P-representations to Entanglement Tests

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To my wife Agnieszka

Do we not do better to recognize that what we call existence consists of countably many iron posts of observation between which we fill in by an elaborate papier-mâché construction of imagination and theory?

John Archibald Wheeler

Abstract

We address the general problem of characterization of states of a quantum system that do not have classical analogs.

At first, we study the long standing problem of characterization of quantumness of states of simple mechanical systems. Using the Galuber-Sudarshan P-representation and the techniques of Fourier transform, we derive a novel family of classicality criteria. For a very broad class of states, these criteria are related to Hilbert's 17th problem: a generic non-classical state can be detected by a polynomial that is a sum of squares of other polynomials. This leads to a natural hierarchy of states regarding their degree of quantumness. Our criteria have the physical meaning of generalized squeezing conditions.

Next, using techniques of harmonic analysis on compact non-Abelian groups, we develop a novel, group-theoretical approach to quantum entanglement of finite dimensional quantum systems. It leads to new reformulations of the separability problem and the positivity of partial transpose (PPT) criterion. When applied to finite groups, our approach allows one to embed the separability problem in a given dimension into a higher dimensional one, but with a high degree of symmetry. We also show a natural connection between the very existence of entanglement and group non-commutativity.

As a by-product, the application of this group-theoretical approach to mechanical systems leads to a unified mathematical language, encompassing both quantum and classical statistics. Within this language, there emerges a novel description of the quantum-to-classical transition at the level of statistics. It originates from the structure of the irreducible representations of the Heisenberg-Weyl group. We also briefly sketch the representation of observables and dynamics in our framework.

Then we study entanglement in multiqubit systems from a more practical point of view. Using the method of entanglement witnesses, we show how to develop novel entanglement tests, formulated as generalized spin squeezing inequalities. Our inequalities provide both necessary and sufficient conditions for genuine 2- and 3-qubit entanglement for symmetric states, and sufficient entanglement conditions for general states. At the same time, the developed inequalities are relatively easily accessible experimentally. Using them, we analyze 7- and 8-ion W-states, recently generated in experiments of the Innsbruck group [Häffner *et al.* Nature **438**, 643 (2005)] and confirm the presence of 2- and 3-qubit entanglement. We also show how to obtain simplified criteria for probing genuine 3-qubit entanglement.

Finally, we develop a system of real polynomial equations describing separable states. We apply to this system methods of classical statistical mechanics: we introduce a canonical ensemble and study the partition function. This leads to an original description of entanglement. For Werner states, our approach generates a sufficient criterion for separability.

Keywords: Entanglement, Harmonic Analysis, Non-classical States

Zusammenfassung

Wir behandeln das Problem der Charakterisierung der jenigen Zustände eines Quantensystems, die keine klassische Entsprechung haben.

Zu Beginn studieren wir im Kontext einfacher mechanischer Systeme das Problem wie man bestimmen kann, in welchem Maße ein Zustand nichtklassisch ist. Mithilfe der Glauber-Sudarshanschen P-Vorteilung und der Fouriertransformation leiten wir eine neue Familie von Kriterien her, die charakterisieren wie klassisch ein Zustand ist. Für eine sehr große Klasse von Zuständen sind diese Kriterien mit Hilberts siebzehntem Problem verwandt: die Quanteneigenschaften solcher Zustände werden durch Polynome nachgewiesen, die jeweils Summe von Quadraten anderer Polynome sind. Dieses führt zu einer natürlichen Hierarchie der Zustände bezüglich ihrer Quanteneigenschaften und Nichtklassizität. Unsere Kriterien können physikalisch als verallgemeinerte Squeezing-Bedingungen interpretiert werden.

Als zweites entwickeln wir eine neuen, gruppentheoretischen Ansatz zur Verschränkung in endlichdimensionalen Quantensystemen, welcher auf harmonischer Analysis nichtkommutativer Gruppen beruht. Dies führt zu einer neuen Formulierung des Separierbarkeitproblems sowie des Kriteriums der Positivität der partiellen Transposition. Auf endliche Gruppen angewendet, erlaubt unser Ansatz, ein gegebenes Separierbarkeitproblems in ein höher-dimensionales hochgradig symmetrisches Separierbarkeitproblem einzubetten. Wir zeigen darüber hinaus eine natürliche Verbindung zwischen Verschränkung und der Nichtkommutativität von Gruppen auf.

Als Nebenprodukt der Anwendung dieses nichtkommutativen Ansatzes bei mechanischen Systemen ergibt sich ein vereinheitlichter mathematischer Formalismus, der sowohl die quantenmechanische als auch die klassische Statistik umfasst. Innerhalb dieses Formalismus entsteht dann eine neue Darstellung der Übergangs zwischen klassischem und quantenmechanischem Regime im Bereich der Statistik. Sie basiert aus der Struktur der irreduziblen Darstellungen der Heisenberg-Weyl Gruppe. Zudem beschreiben wir kurz die Darstellung von Observablen sowie der Dynamik in diesem Formalismus.

Dann studieren wir noch die Verschränkung in Multiqubitsystemen aus einem praktischeren Blickwinkel. Mit der Methode der Verschränkungs- zeigen wir, wie neue Verschränkungskriterien entwickelt werden können, die als verallgemeinerte Spin-Squeezing Ungleichungen formuliert sind. Unsere Ungleichungen liefern sowohl

notwendige als auch hinreichende Bedingungen für echte Zwei- und Dreiqubitverschränkung symmetrischer Zustände, sowie hinreichende Verschränkungsbedingungen für allgemeine Zustände. Experimentell sind diese Ungleichungen zudem relativ einfach zugänglich. Wir benutzen sie dann, um die kürzlich in Innsbruck experimentell erzeugten 7- und 8-Ionen Werner Zustände [Häffner et al. Nature **438**, 643 (2005)] zu analysieren. Dabei weisen wir Zwei- und Dreiqubitverschränkung nach. Ferner zeigen wir, wie vereinfachte Kriterien entwickelt werden können, um echte Dreiqubitverschränkung nachzuweisen.

Als letztes entwickeln wir ein System reeller polynomieller Gleichungen, die separierbare Zustände beschreiben. Wir schlagen daraufhin vor, auf dieses System Methoden der klassischen statistischen Mechanik anzuwenden, führen ein kanonisches Ensemble ein und studieren die Zustandssumme. Dies wiederum führt zu einer neuen Beschreibung der Verschränkung, die für Wernerzustände ein hinreichendes Kriterium der Separierbarkeit liefert.

Schlagwörter: Verschränkung, Harmonische Analysis, Nichtklassische Zustände

Contents

Chapter 1

General introduction

1.1 Motivation and the levels of influence

The problem of quantumness, understood as a characterization of those exclusive features of quantum systems, which have no analogs in the classical world, has been addressed by several generations of physicists from the very beginning of quantum theory. One of the first, most pronounced, and most widely recognized example of such a quantum feature has been the non-commutativity of observables in quantum mechanics, leading to the famous Heisenberg uncertainty relations. Another one is the principle of linear superposition, manifesting itself e.g. in interference experiments not only with neutrons or electrons, but also with fullerenes and even hemoglobin molecules. Yet another genuinely quantum feature is quantum entanglement, which has been puzzling and exciting physicists since its discovery in 1935 by Einstein, Podolsky, and Rosen [22] and Schrödinger [89]. For an overview see e.g. Wheeler and Żurek [106] and Peres [73].

Generally, we can speak about the problem of quantumness at four different levels. At the deepest, philosophical level, the works of Einstein (see Schilpp [86]) and Bell [5] brought to the light the fact that we still do not know the answers to several fundamental questions: What is reality? What are the basic constituents of our world? Matter? Fields? Information? Is our description of the world complete? If not, what theory underlines it? Is this theory quantum or classical?

The last questions, lying at the border between philosophy and physics, bring us to the next level — the fundamentals of physics. At this level, physicists are still looking for the right "interpretation", or "derivation" of quantum mechanics. In our opinion, the problem of quantumness is of a great importance here. For example, theoretical proofs of existence followed by experimental observations of quantum states without classical analogs, like entangled states, squeezed states, etc, serve the vital purpose of proving that the necessarily statistical description of the world provided by quantum mechanics is *not* a special case of classical statistics. The ability to characterize and prepare physical systems in genuinely quantum states is the necessary prerequisite for accessing and hopefully comprehending those, seemingly by

definition, counterintuitive features of quantum mechanics. Another influence of the problem of quantumness at the very foundations of physics (and not only) has been developing in the past 15 years or so with the discovery of quantum information; see e.g. Nielsen and Chuang [70]. Although this notion is still not precisely formulated, there has been attempts to treat information and its processing as the fundamental building block of the observed world.

The efficient description of quantum states connects us to the next level — the level of mathematics. Practical characterization of quantum states is by no means an easy task. The most difficult example, which has so far resisted all the attempts of resolution, is the problem of efficient description of entangled states, know as the *separability problem*. Posed relatively recently, compared to the first works on entanglement, by Werner [102] it touches some open problems in mathematics, e.g. the characterization of positive but not completely positive maps; see Størmer [95] and Woronowicz [110]. We may hope that the problem of quantumness in general, or the separability problem in particular, will stimulate a development of new methods or even new branches of mathematics, just like several other physical problems did.

The final level is the level of practical applications of the problem of quantumness. Quite recently scientists and engineers have realized that most of the "weird" features of quantum mechanics can actually be practically employed. Since the ground breaking theoretical works and experiments on quantum computation, teleportation, quantum dense coding, and quantum cryptography it became clear that there is a way to bring quantum mechanics to the technological level (for more details see e.g. Bouwmeester *et al.* [8]). The most developed in this respect area is that of quantum cryptography, where at the present day at least two commercial companies offer cryptographic devices, allowing for super-secure communication over dozens of kilometres. For all those practical applications, relying solely on genuine quantum states, the ability of efficient, on-the-flight recognition of genuine quantum statistics is of the fundamental importance.

1.2 This work

The purpose of (a big part of) this work is to show that a one particularly interesting framework for studying quantumness is provided by the Fourier transform and its generalizations. The method proposed by Jean Baptiste Joseph Fourier in his fundamental work *Théorie Analytique de la Chaleur*, published in Paris in 1822 [25], has found so far an application in an amazingly wide spectrum of areas — from foundations of mathematics (harmonic analysis and non-commutative geometry) to hardware implementation in chips, for example performing voice recognition. In the basic quantum mechanics, Fourier transform connects coordinate-space and momentum-space descriptions of a mechanical system. It this work we apply it, and its generalizations, to the several aspects of the quantumness problem. We provide here only a general overview. More detailed descriptions, together with all the related definitions, follow in the first sections of each Chapter.

We begin with showing how standard Fourier transform and Glauber-Sudarshan P-representation can be used for solving the problem of quantumness of states of a simple mechanical system, like a harmonic oscillator. The main result of this investigation is that for a wide class of states, genuine quantum states are completely described by polynomials in creation and annihilation operators, which are sums of squares (SOS) of other polynomials. This essentially generalizes the standard notions of squeezing, used for decades in quantum optics. At the mathematical level, our solution is related to Hilbert's 17th problem — one of the fundamental problems in real algebra.

Next, we apply the generalization of the Fourier transform to compact, non-Abelian groups for analyzing entanglement in finite dimensional systems. We reformulate and generalize the separability problem in group-theoretical terms, which in itself constitutes an interesting and novel mathematical problem. We show how some of the known methods of entanglement study can be translated into this new language and allow one to make highly non-trivial statements concerning positive definite functions on compact non-Abelian groups. When applied to finite groups, like groups of permutations, our formalism connects separability problems in different dimensions. In the broader context of non-commutative geometry, our methods can be viewed as a way of analyzing non-commutative probabilistic measures.

Application of the above approach to the non-compact Heisenberg-Weyl group leads to a modification of the standard Weyl quantization, within which both quantum and classical statistics are described in a very uniform way. The main feature of the resulting language is an elegant and natural description of the transition from quantum to classical regime.

On a more practical side, we approach a problem of characterization, in an experimentally accessible way, of multipartite entanglement. We analyze a system of qubits, i.e. the simplest quantum systems described by $\mathbb{C}^2$, from a novel perspective and show how to describe multiqubit entanglement through certain conditions on the fluctuations of the total spin. This conditions are given in a form of inequalities, generalizing the standard notion of spin squeezing. For symmetric states, this inequalities provide both necessary and sufficient criteria for genuine 2- and 3-qubit entanglement, while for general states they serve as sufficient 2- and 3-qubit entanglement criteria. At the mathematical level, this approach is related to characterization of probabilistic measures on a homogeneous space, which in this case is a sphere. To emphasize the experimental importance of our approach, we apply it to a concrete experimental output of a recent experiment, aimed at producing states suitable for quantum computation (Häffner *et al.* [36]).

In the only part of the work not connected to the Fourier transform, we apply classical-statistical methods to the analysis of a real system of polynomials describing separable states. For the system of polynomial equations, we define a canonical partition function and numerically study its properties for Werner states. The proposed approach can be treated as an example of a "statistical real algebra" and is a novel way of looking at the entanglement.

The work is organized as follows. In Chapter 2 we address the problem of

quantumness of states of a mechanical system and connect it with Hilbert's 17th problem. In Chapter 3 we present a short introduction into the separability problem and then proceed with its reformulation using non-commutative Fourier transform. Chapter 4 is dedicated to the description of the correspondence principle, using the formalism of Chapter 3. In Chapter 5 we derive the generalized spin squeezing inequalities. Finally, in Chapter 6 we present the statistical-mechanical approach to studying entanglement.

Chapter 2

Quantumness of states of a mechanical system

This Chapter is dedicated to an analysis of quantumness of states of a simple mechanical system, such as a harmonic oscillator. First, we address the mathematical problem of existence of the, so called, Glauber-Sudarshan P-representation, which is the basic tool for studying quantumness. Then, we derive a family of classicality criteria that require that averages of positive functions calculated using the P-representation must be positive. For a large class of states, these criteria are related to Hilbert's 17th problem, and have a physical meaning of generalized squeezing conditions; alternatively, they may be interpreted as *non-classicality witnesses*. We show that every generic non-classical state can be detected by a polynomial that is a sum of squares of other polynomials (SOS). This leads to a natural hierarchy of states regarding their degree of quantumness, which we relate to the minimal degree of a SOS polynomial that detects them. Finally, we discuss the significance of our results for general mechanical systems and the experimental implementability of the polynomial non-classicality witnesses.

2.1 Definition of the problem

The problem of existence of a classical probabilistic description of quantum states of a mechanical system has a long history and can be traced back to the seminal papers of Glauber [29] and Sudarshan [96]. Before we define what we exactly mean by quantumness of states, we need to introduce some notions.

Let us consider a one dimensional mechanical system, described by a Hilbert space $L^2(\mathbb{R})$ with a fixed basis of Fock states $|n\rangle$. Let us also fix the canonical annihilation and creation operators a, $a^\dagger$. Then, in the works of Glauber [29] and Sudarshan [96] it was shown that any state ϱ our system can be uniquely put into a form diagonal in the coherent states $|\alpha\rangle$:

$$\varrho = \int_{\mathbb{R}^2} \mathrm{d}^2\alpha \, P_\varrho(\alpha, \overline{\alpha}) |\alpha\rangle\langle\alpha| \,, \tag{2.1}$$

where $\alpha = (1/\sqrt{2\hbar})(\xi + \mathrm{i}\eta)$ is the coherence parameter, $\mathrm{d}^2\alpha := \mathrm{d}\xi\mathrm{d}\eta/2\hbar$, and bar denotes complex conjugation. The decomposition (2.1) is called the Glauber-Sudarshan P-representation (or simply the P-representation) of the state ϱ. The exact mathematical meaning of the integral in Eq. (2.1) will be clarified in the next Section.

Now we are ready to give the following, standard (see e.g. Mandel and Wolf [65]) definition:

Definition 2.1. *A state ϱ is called classical with respect to measurements of a given set of canonical observables if the Glauber-Sudarshan P-representation from Eq. (2.1) defines a positive phase-space probability distribution.*

Mathematical speaking, for classical states, P_ϱ defines a probabilistic measure μ_ϱ on the classical phase-space $\mathbb{R}^2$ through:

$$\mathbb{R}^2 \supset \Omega \mapsto \mu_\varrho(\Omega) := \int_\Omega \mathrm{d}^2\alpha \, P_\varrho(\alpha, \overline{\alpha}) \geq 0 \,. \tag{2.2}$$

Recall that a Borel measure μ on a space X is called *probabilistic* if it is positive, i.e. $\mu(\Omega) \geq 0$ for any Borel set Ω, and normalized: $\mu(X) = 1$. Statistical properties of a state possessing positive P-representation are as those of a classical statistical ensemble, described by the measure μ_ϱ; that explains why such states are called *classical*.

However, the class of allowed P_ϱ's is larger than that, as we will show in the next Section, and there exist states (such as squeezed states, or Fock states) for which the integral (2.2) does not always exist, or attains negative values. Such states will be called *genuine quantum*. A natural problem arises: given a state ϱ decide weather it is classical or genuine quantum.

Geometrically, the set of all probabilistic measures forms a convex subset of the set of all P_ϱ's. The extreme points of this set are the point-concentrated measures $\{\delta^2(\alpha - \beta); \beta \in \mathbb{C}\}$, corresponding to pure coherent states $|\alpha\rangle\langle\alpha|$. A decomposition of any measure into these points is unique, since Dirac's δ is a unique unit element with respect to the convolution: $P(\alpha, \overline{\alpha}) = \int \mathrm{d}^2\beta P(\beta, \overline{\beta})\delta^2(\alpha - \beta)$. Hence, classical states form a generalized simplex Δ. This is a general feature of a set of probabilities describing classical systems, as emphasized by Mielnik in Ref. [66]. Therefore, in geometrical language the problem of distinguishing between classical and genuine quantum states amounts to the operational description of the simplex of positive measures Δ in the space of all P_ϱ's. The closely related problem occurs in the study of quantum entanglement, to which the next Chapters are devoted, with the difference that the convex subset of classically correlated states is not a simplex. Before developing the method of solving the quantumness problem, we first have to put the integral (2.1) into a rigorous mathematical form.

2.2 Existence of the P-representation

2.2.1 Coherent states

First of all, we will need some basic properties of coherent states $|\alpha\rangle$. We simply quote them here, referring the reader to the standard book of Perelomov [72] for more details. Traditionally, coherent states are defined and used for systems with quadratic Hamiltonians, but they can also be defined purely kinematically, i.e. without any reference to a concrete mechanical system, a concrete basis in the Hilbert space, etc. We shall do so here and define coherent states as the states that minimize the Heisenberg uncertainty relations:

$$\Delta q \Delta p = \frac{\hbar}{2} \tag{2.3}$$

with isotropic distribution of the uncertainties in the phase-space. Equivalently, they can be defined as the eigenstates of the annihilation operator:

$$a|\alpha\rangle = \alpha|\alpha\rangle. \tag{2.4}$$

Yet another useful definition is obtained using Weyl operators:

$$W(\xi,\eta) := \exp\Big[-\frac{\mathrm{i}}{\hbar}(\xi\hat{p} - \eta\hat{q})\Big]. \tag{2.5}$$

We exceptionally put the hat over the position and momentum operators $\hat{q}$ and $\hat{p}$ in order to avoid any confusions with the classical phase-space coordinates (q,p). We will study Weyl operators in more detail in Chapter 4, where it will become clear why we label $W(\xi,\eta)$ by some parameters (ξ,η) rather than directly by the coordinates (q,p). Using the operators (2.5), coherent states can be defined as follows:

$$|\alpha\rangle := W(\alpha)|0\rangle, \quad \alpha := \frac{1}{\sqrt{2\hbar}}(\xi + \mathrm{i}\eta), \tag{2.6}$$

where $|0\rangle$ is the Fock's ground state. It can be alternatively defined as the unique coherent state with the property $\langle\hat{q}\rangle = \langle\hat{p}\rangle = 0$. From Eq. (2.6) it is easy to see that in the basis of Fock states $|n\rangle$, the coordinates of $|\alpha\rangle$ read:

$$|\alpha\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}} \sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \tag{2.7}$$

From either Eq. (2.6) or Eq. (2.7), it follows that that coherent states are not mutually orthogonal and satisfy:

$$\langle\alpha|\beta\rangle = \exp\left(-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2 + \overline{\alpha}\beta\right). \tag{2.8}$$

This leads us to the next property: coherent states form an overcomplete system in $L^2(\mathbb{R})$. That is, they span the whole space:

$$\int_{\mathbb{R}^2} \frac{\mathrm{d}^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = \mathbf{1}, \tag{2.9}$$

but the cardinality of the set $\{|\alpha\rangle; \alpha \in \mathbb{C}\}$ is too high (continuum), since $L^2(\mathbb{R})$ is separable and possesses a countable basis (like the basis given by Fock states). It is a very remarkable result that a complete subsystem, i.e. a basis of $L^2(\mathbb{R})$, is obtained by taking a subset $\{|\alpha_{mn}\rangle; m, n \in \mathbb{N}\}$, corresponding to a lattice in $\mathbb{R}^2$ with an elementary cell area equal to π (or $2\pi\hbar$ in the phase-space related coordinates (ξ, η) from Eq. (2.5)). Thus, heuristically speaking, classical phase-space contains in some sense redundant continuum structure, but on the other hand does not support the right, information-wise, structure: the linear superpositions of states.

2.2.2 Proof of existence of the P-representation

The overcompletness of coherent states has a very interesting implication. Namely, we show, following Miller and Mishkin [67], that the following fact holds:

Theorem 2.1. *For every trace-class operator A on $L^2(\mathbb{R})$ there exists a unique distribution P_A from a suitable class of distributions, such that A can be represented as:*

$$A = \int_{\mathbb{R}^2} d^2\alpha \, P_A(\alpha, \overline{\alpha}) |\alpha\rangle\langle\alpha| \,, \tag{2.10}$$

in the sense of matrix elements.

Recall that an operator A is called trace-class if its trace norm $||A||_1 := \mathrm{tr}\sqrt{A^\dagger A}$ is finite. One notational remark: we interchangeably treat appearing functions as either functions on $\mathbb{R}^2$, or as functions on $\mathbb{C}$.

Proof. The basic idea is to treat Eq. (2.10) as a formal expression and first prove the existence of the Fourier transform of P_A. In this Chapter, the Fourier transform of a function f is defined as follows:

$$\mathcal{F}f(z, \overline{z}) := \int \mathrm{d}^2\alpha f(\alpha, \overline{\alpha}) \mathrm{e}^{z\overline{\alpha} - \overline{z}\alpha}, \tag{2.11}$$

while the inverse transform is given by:

$$\mathcal{F}^{-1}f(\alpha, \overline{\alpha}) = \int \frac{4\mathrm{d}^2 z}{\pi^2} f(z, \overline{z}) \mathrm{e}^{-z\overline{\alpha} + \overline{z}\alpha} \,. \tag{2.12}$$

From Eqs. (2.10) and (2.11) it formally follows that:

$$\mathcal{F}P_A(z, \overline{z}) = \mathrm{tr}[A :W(z):] = \mathrm{e}^{\frac{|z|^2}{2}} \mathrm{tr}[A\, W(z)], \tag{2.13}$$

where the colons : : denote the normal ordering:

$$:W(z): = \mathrm{e}^{za^\dagger} \mathrm{e}^{-\overline{z}a} = \mathrm{e}^{\frac{|z|^2}{2}} W(z) \tag{2.14}$$

and we used the formula $\mathrm{e}^{A+B} = \mathrm{e}^{-\frac{1}{2}[A,B]} \mathrm{e}^A \mathrm{e}^B$ above. When A is a density matrix, i.e. when $A = \varrho$, the following definition holds:

Definition 2.2. *Function $\mathcal{F}P_\varrho$ is called a characteristic function of the state ϱ.*

We will study characteristic functions of states and their ramifications more closely in Chapters 3 and 4. Observe that since A is trace-class and $W(z)$ is unitary for any z, the right hand side of Eq. (2.13) is a well defined function and so is $\mathcal{F}P_A$. Equivalently $\mathcal{F}P_A$ can be obtained from the, so called, *Q-representation* of A:

$$A(\alpha, \overline{\alpha}) := \langle \alpha | A \alpha \rangle \,, \tag{2.15}$$

which is formally related to the P-representation through:

$$A(\beta, \overline{\beta}) = \int_{\mathbb{R}^2} \mathrm{d}^2\alpha \, P_A(\alpha, \overline{\alpha}) \, \mathrm{e}^{-|\alpha-\beta|^2} \,. \tag{2.16}$$

Applying the Fourier transform (2.11) to Eq. (2.16), one obtains:

$$\mathcal{F}P_A(z, \overline{z}) = \frac{1}{\pi} \, \mathrm{e}^{|z|^2} \, \mathcal{F}A(z, \overline{z}). \tag{2.17}$$

Now the whole difficulty is to invert the Fourier transform in a suitable sense. For that, we first examine the properties of $\mathcal{F}P_A$, implied by Eq. (2.13). By diagonalizing $W(z)$, $W(z) = \sum_j \mathrm{e}^{\mathrm{i}\varphi_j(z)} |\psi_j(z)\rangle\langle\psi_j(z)|$, and using the Schwarz inequality:

$$|\langle \psi_1 | \psi_2 \rangle| \leq ||\psi_1|| \, ||\psi_2||, \tag{2.18}$$

we obtain the following bound:

$$\big|\mathrm{tr}[A \, W(z)]\big|^2 \leq \sum_j \big|\langle \psi_j(z) | A \psi_j(z) \rangle\big|^2 \leq \sum_j ||A\psi_j(z)||^2 = ||A||_2{}^2 \,, \tag{2.19}$$

where $||A||_2 := \sqrt{\mathrm{tr}(A^\dagger A)}$ is the Hilbert-Schmidt norm of A. The strong continuity of $W(z)$ with respect to z implies that:

$$\begin{aligned} &\Big|\mathrm{tr}\big(A \, [W(z) - W(z')]\big)\Big|^2 \leq \sum_n \Big|\langle A^\dagger n | [W(z) - W(z')] n \rangle\Big|^2 \\ &\leq \sum_n ||A^\dagger n||^2 \, ||[W(z) - W(z')]n||^2 \leq C^2 |z - z'|^2 \, \mathrm{tr}(AA^\dagger) \\ &= C^2 ||A||_2{}^2 |z - z'|^2 \end{aligned} \tag{2.20}$$

for some constant C. Hence, $\mathcal{F}P_A$ is a continuous function bounded by:

$$|\mathcal{F}P_A(z, \overline{z})| \leq ||A||_2{}^2 \, \mathrm{e}^{\frac{|z|^2}{2}} \,. \tag{2.21}$$

It does not have to be differentiable, as $\mathrm{tr}[A \, a \, W(z)]$ and $\mathrm{tr}[A \, a^\dagger \, W(z)]$ may not exist, because the operators $a, a^\dagger$ are unbounded.

Due to the bond (2.21), $\mathcal{F}P_A$ can grow very rapidly and hence one cannot simply apply the inverse functional transform (2.12) to it. A way to invert the Fourier transform in Eq. (2.13) is to treat $\mathcal{F}P_A$ as a distribution itself — for any function χ with a compact support, the integral:

$$\langle \mathcal{F}P_A, \chi \rangle := \int \mathrm{d}^2 z \, \mathcal{F}P_A(z, \overline{z}) \chi(z, \overline{z}) \tag{2.22}$$

is well defined and finite. The space of test functions with compact supports, equipped with the proper topology, is standardly denoted by $\mathcal{D}(\mathbb{R}^2)$. We refer the reader to Gel'fand and Shilov [26] or Reed and Simon vol. 2 [76] for the detailed exposition of the theory of distributions. Hence, $\mathcal{F}P_A$ can be treated as an element of the dual distribution space $\mathcal{D}'(\mathbb{R}^2)$.

Formally, from the definition of the Fourier transform on distributions, we can define P_A through:

$$\langle P_A, \mathcal{F}\chi\rangle := \langle \mathcal{F}P_A, \chi\rangle\,. \tag{2.23}$$

To make the above expression meaningful, one has to find the image $\mathcal{F}(\mathcal{D}(\mathbb{R}^2))$ of $\mathcal{D}(\mathbb{R}^2)$ under the Fourier transform. For that, note that the Fourier transform of any $\chi \in \mathcal{D}(\mathbb{R}^2)$:

$$\mathcal{F}\chi(\alpha,\overline{\alpha}) = \int \mathrm{d}^2\alpha\, \chi(z,\overline{z})\mathrm{e}^{\overline{z}\alpha - z\overline{\alpha}} \tag{2.24}$$

can be analytically continued to an entire function on $\mathbb{C}^2$, i.e. to a function holomorphic on the whole space, by substituting $\mathrm{Re}\alpha$ and $\mathrm{Im}\alpha$ with complex variables (ζ_1,ζ_2). The integral (2.24) is still well defined after such a substitution, due to the compact support of χ. Let us call this continuation $(\mathcal{F}\chi)^{\mathbb{C}}$. Then one proves easily by brutally substituting functions with their suprema over $\mathrm{supp}\chi$ that the following bound holds:

$$\left|\zeta_1^k\,\zeta_2^l\,(\mathcal{F}\chi)^{\mathbb{C}}(\zeta_1,\zeta_2)\right| \leq c_{k,l}\exp(b_1|\mathrm{Im}\zeta_1| + b_2|\mathrm{Im}\zeta_2|) \tag{2.25}$$

for any natural k,l and for some positive constants $c_{k,l}, b_1$, and b_2.

The converse is also true: any entire function on $\mathbb{C}^2$ satisfying the above condition is of the form $(\mathcal{F}\chi)^{\mathbb{C}}$ for some $\chi \in \mathcal{D}(\mathbb{R}^2)$. This is the, so called, Paley-Wiener Theorem (see e.g. Gel'fand and Shilov vol. 1 [26] or Reed and Simon vol 2. [76]). The space of entire functions satisfying the bond (2.25) and equipped with the topology of almost uniform convergence on the real plane only, is standardly denoted by $\mathcal{Z}(\mathbb{C}^2)$. Thus, from Eq. (2.23) follows that P_A is defined on functions, which are restrictions to $\mathbb{R}^2$ of functions form $\mathcal{Z}(\mathbb{C}^2)$. The restriction is obtained by setting to zero the imaginary parts of the coordinates (ζ_1,ζ_2) (this is what we mean by the real plane). We will denote the space of such functions by $\mathcal{Z}(\mathbb{R}^2)$. Hence, by Eq. (2.23) P_A is a distribution from the dual space[1] $\mathcal{Z}'(\mathbb{R}^2)$, sometimes called the space of ultradistributions on $\mathbb{R}^2$.

Due to Eq. (2.16), the above constructed distribution P_A reproduces only the diagonal elements $\langle\alpha|A\alpha\rangle$. We now have to show that they determine the operator A completely. Following Perelomov [72], consider a function:

$$\widetilde{A}(\overline{\alpha},\beta) := \exp\left(\frac{|\alpha|^2+|\beta|^2}{2}\right)\langle\alpha|A\beta\rangle. \tag{2.26}$$

Completeness of coherent states implies that $\widetilde{A}(\overline{\alpha},\beta)$ determines A completely. It is an entire function of $(\overline{\alpha},\beta)$, as can be seen from Eq. (2.7), and obviously remains such

[1] Note that P_A can be prolonged to a distribution $P_A^{\mathbb{C}} \in \mathcal{Z}'(\mathbb{C}^2)$ by the following prescription: $\langle P_A^{\mathbb{C}}, (\mathcal{F}\chi)^{\mathbb{C}}\rangle := \langle P_A, \mathcal{F}\chi\rangle\,.$

in the rotated coordinates $u := (\overline{\alpha} + \beta)/2$, $v := \mathrm{i}(\overline{\alpha} - \beta)/2$. But any entire function is completely determined by its values at a real plane, which in the new coordinates (u, v) corresponds to $\alpha = \beta$. Thus, $\widetilde{A}(\overline{\alpha}, \beta)$ is completely determined by its diagonal values $\widetilde{A}(\alpha, \overline{\alpha})$ and so is the function $\langle\alpha|A\beta\rangle = \exp\left[-(|\alpha|^2 + |\beta|^2)/2\right] \widetilde{A}(\overline{\alpha}, \beta)$. Hence, every operator A is completely determined by its Q-representation $\langle\alpha|A\alpha\rangle$.

To proof uniqueness, let P_A and P'_A both correspond to the same operator A. By taking coherent-state diagonal matrix elements (which as we know are enough), we obtain that:

$$\int \mathrm{d}^2\alpha (P_A - P'_A)|\alpha\rangle\langle\alpha| = 0 \quad \text{if and only if} \int \mathrm{d}^2\alpha (P_1 - P_2)\mathrm{e}^{-|\alpha-\beta|^2} = 0 \tag{2.27}$$

for all $\beta \in \mathbb{C}$. The Fourier transform of the last equation yields $\mathcal{F}P_A = \mathcal{F}P'_A$, which is satisfied if and only if $P_A = P'_A$. □

Thus, we see that indeed every trace-class operator possesses the representation (2.10), provided that one allows for the distributive P-representations from a suitably broad class of distributions. Nevertheless, in the physical literature P_A is often called the "P-function", although the more appropriate name would be the "P-distribution". Also, the corresponding "function-like" notation is commonly used, i.e. $P_A(\alpha, \overline{\alpha})$, etc. We will stick to that traditional notation too, in particular we will write the P-representation in the form (2.10), but it should be kept in mind that such integrals are understood in the above distributive sense.

2.2.3 Some remarks

Some more general remarks are in order. Note that $\mathcal{F}P_A$ is a rather specific element of the distribution space $\mathcal{D}'(\mathbb{R}^2)$, as it is a continuous function satisfying the condition (2.21). Thus, $\mathcal{F}P_A$ can act on a wider class of functions than $\mathcal{D}(\mathbb{R}^2)$ and therefore P_A can also be defined on a larger space than $\mathcal{Z}(\mathbb{R}^2)$. However, the explicit description of this spaces does not seem, up to our knowledge, to exist.

So far we have been considering general trace-class operators A. For density matrices ϱ their P-representations P_ϱ possess some additional properties. Hermiticity and normalization imply that:

$$\overline{P_\varrho} = P_\varrho, \quad \int \mathrm{d}^2\alpha\, P_\varrho(\alpha, \overline{\alpha}) = 1, \tag{2.28}$$

while positivity implies that for every vector $|\psi\rangle$ it holds:

$$\int \mathrm{d}^2\alpha\, P_\varrho(\alpha, \overline{\alpha})|\langle\alpha|\psi\rangle|^2 \geq 0. \tag{2.29}$$

It is straightforward to see that probabilistic measures on the phase-space $\mathbb{R}^2$ satisfy the above conditions. However, the space of all allowed P_ϱ's is much larger than that, since the Fourier transform of a probabilistic measure μ, i.e. its classical characteristic function (see e.g. Abramowitz and Stegun [1]):

$$\mathcal{F}\mu(z, \overline{z}) := \int \mathrm{d}\mu(\alpha, \overline{\alpha})\mathrm{e}^{z\overline{\alpha} - \overline{z}\alpha} \tag{2.30}$$

satisfies $|\mathcal{F}\mu(z,\overline{z})| \leq 1$, while from Eq. (2.21) it follows that the characteristic function of a state, $\mathcal{F}P_\varrho$, satisfies only a less restrictive condition:

$$|\mathcal{F}P_\varrho(z,\overline{z})| \leq \mathrm{e}^{\frac{|z|^2}{2}}. \tag{2.31}$$

An interesting example of how singular P_ϱ can be due to the above bond, is provided by the P-representation of a superposition of two coherent states $|\psi\rangle := c_1|\alpha\rangle + c_2|\beta\rangle$:

$$\begin{aligned}
P_\psi(\gamma,\overline{\gamma}) &= |c_1|^2\delta^2(\gamma-\alpha) + |c_2|^2\delta^2(\gamma-\beta) \\
&+ c_1\overline{c_2}\exp\Big(|\gamma|^2 - \frac{|\alpha|^2}{2} - \frac{|\beta|^2}{2}\Big)\exp\left(\frac{\overline{\alpha}-\overline{\beta}}{2}\frac{\partial}{\partial(\overline{\gamma}-\frac{\overline{\alpha}}{2}-\frac{\overline{\beta}}{2})}\right) \\
&\times\exp\left(\frac{\beta-\alpha}{2}\frac{\partial}{\partial(\gamma-\frac{\alpha}{2}-\frac{\beta}{2})}\right)\delta^2\Big(\gamma-\frac{\alpha}{2}-\frac{\beta}{2}\Big) \\
&+ \overline{c_1}c_2\exp\Big(|\gamma|^2 - \frac{|\alpha|^2}{2} - \frac{|\beta|^2}{2}\Big)\exp\left(\frac{\overline{\beta}-\overline{\alpha}}{2}\frac{\partial}{\partial(\overline{\gamma}-\frac{\overline{\alpha}}{2}-\frac{\overline{\beta}}{2})}\right) \\
&\times\exp\left(\frac{\alpha-\beta}{2}\frac{\partial}{\partial(\gamma-\frac{\alpha}{2}-\frac{\beta}{2})}\right)\delta^2\Big(\gamma-\frac{\alpha}{2}-\frac{\beta}{2}\Big),
\end{aligned} \tag{2.32}$$

where $\delta^2(\alpha) := \delta(\mathrm{Re}\alpha)\delta(\mathrm{Im}\alpha)$. We see that P_ψ involves infinite-order derivatives of the Dirac's delta function.

2.3 General solution

After the necessary mathematical introduction, we present a general method of detecting genuine quantum states based on Bochner's Theorem. The method was first introduced in our work [50].

The starting point is the solution of the quantumness problem, proposed by Richter and Vogel in Ref. [78] (see also Shchukin and Vogel [90]). For a given state ϱ, they studied the characteristic function of ϱ, i.e. the Fourier transform $\mathcal{F}P_\varrho$ defined by Eq. (2.13). The criterion detecting probabilistic measures is then provided by Bochner's Theorem:

Theorem 2.2 (Bochner). *$\mathcal{F}P_\varrho$ is the Fourier transform of a probabilistic measure if and only if $\mathcal{F}P_\varrho$ is a positive definite function, i.e. for all n and all sequences $\xi_1,\ldots,\xi_n \in \mathbb{R}^2$ the $n\times n$ matrix $\boldsymbol{P}_{\varrho ij} := \mathcal{F}P_\varrho(\xi_i-\xi_j)$ is positive semidefinite[2] and $\boldsymbol{P}_{\varrho ii} = 1$.*

The proof in one direction follows trivially from the Eq. (2.30). The implication in the other direction is much more difficult to show and we will not do it here, referring the reader to e.g. Reed and Simon vol. 2 [76] or Folland [24]. Let us

[2]For compactness, we did not indicate explicitly the dependence of $\mathcal{F}P_\varrho$ on the complexly conjugate parameters. Whenever it is done in the sequel, this dependence is understood.

also note that a more general form of this Theorem will be shown in Section 3.7 of Chapter 3.

The further test of $\boldsymbol{P}_\varrho$ being positive semidefinite for a fixed sequence $\xi_1, \ldots, \xi_n$ is carried out by using the determinant criterion: $\boldsymbol{P}_\varrho$ is positive semidefinite if and only if the determinants D_k, $k = 1 \ldots n$ of all of the principal submatrices of $\boldsymbol{P}_\varrho$ are non-negative. This finally leads to the hierarchy of conditions: a state ϱ is nonclassical if and only if there exist $k > 2$ (for $k = 1$, $D_1 = 1$ due to the normalization) and a sequence $\xi_1, \ldots, \xi_k \in \mathbb{R}^2$, such that $D_k < 0$.

The starting point of our approach is the observation that the positive definiteness condition from Theorem 2.2 can be equivalently (for continuous functions; see Folland [24]) defined in the following way, which we will use extensively in the next Chapters:

Definition 2.3. *A bounded function ϕ on $\mathbb{R}^n$ is called positive definite if:*

$$\iint d^n\boldsymbol{x}\, d^n\boldsymbol{y}\, \overline{f(\boldsymbol{x})}\phi(\boldsymbol{x}-\boldsymbol{y})f(\boldsymbol{y}) \geq 0 \quad \textit{for any } f \in L^1(\mathbb{R}^n). \tag{2.33}$$

Moreover, since functions with compact support are dense in $L^1(\mathbb{R}^n)$, we can equivalently use them in the definition (2.33). As a consequence, the necessary and sufficient condition for P_ϱ to define a probabilistic measure through Eq. (2.2) is that:

$$\iint \mathrm{d}^2z\, \mathrm{d}^2z'\, \overline{\chi(z)}\ \mathcal{F}P_\varrho(z-z')\ \chi(z') \geq 0 \quad \text{for any } \chi \in \mathcal{D}(\mathbb{R}^2). \tag{2.34}$$

From the definition of Fourier transform (2.11), the above integral can be rewritten as follows:

$$\begin{aligned}
&\iiint \mathrm{d}^2z\, \mathrm{d}^2z'\mathrm{d}^2\alpha\, \overline{\chi(z)}\chi(z') \exp\big[(z-z')\overline{\alpha} - (\overline{z}-\overline{z}')\alpha\big] P_\varrho(\alpha) \\
&= \int \mathrm{d}^2\alpha \left(\int \mathrm{d}^2z'\chi(z')\mathrm{e}^{\alpha\overline{z}'-\overline{\alpha}z'} \right) \overline{\left(\int \mathrm{d}^2z\chi(z)\mathrm{e}^{\alpha\overline{z}-\overline{\alpha}z} \right)}\, P_\varrho(\alpha) \\
&= \int \mathrm{d}^2\alpha P_\varrho(\alpha) |\mathcal{F}\chi(\alpha)|^2.
\end{aligned} \tag{2.35}$$

But from the Paley-Wiener Theorem (see Eq. (2.25) and the following paragraph), we know that $\mathcal{F}\chi \in \mathcal{Z}(\mathbb{R}^2)$ and any function from $\mathcal{Z}(\mathbb{R}^2)$ is of that form. Recall that $\mathcal{Z}(\mathbb{R}^2)$ are the restrictions to $\mathbb{R}^2$ of the functions from $\mathcal{Z}(\mathbb{C}^2)$, i.e. the space of entire functions on $\mathbb{C}^2$ satisfying the condition (2.25). Hence, we obtain the following criterion for classicality:

Theorem 2.3. *A state ϱ is classical if and only if:*

$$\int d^2\alpha\, P_\varrho\, |f_{\mathbb{R}}|^2 \geq 0 \quad \textit{for any} \quad f \in \mathcal{Z}(\mathbb{C}^2), \tag{2.36}$$

where $f_{\mathbb{R}}$ denotes the restriction of f to $\mathbb{R}^2$, obtained by setting to zero the imaginary parts of the arguments.

The only thing we have to ensure is that the integral (2.36) is well defined. Since $P_\varrho \in \mathcal{Z}'(\mathbb{R}^2)$, one has to show that $|f_\mathbb{R}|^2$ belongs to $\mathcal{Z}(\mathbb{R}^2)$, i.e. there exists $g \in \mathcal{Z}(\mathbb{C}^2)$, such that $g_\mathbb{R} = |f_\mathbb{R}|^2$. By Paley-Wiener theorem $f = (\mathcal{F}\chi)^\mathbb{C}$ for some $\chi \in \mathcal{D}(\mathbb{R}^2)$. Define $g := |(\mathcal{F}\chi)^\mathbb{C}|^2$. Then, $g_\mathbb{R} = |f_\mathbb{R}|^2$ and from (2.25): $|\zeta_1^k \zeta_2^l g(\zeta_1, \zeta_2)| = |(\mathcal{F}\chi)^\mathbb{C}| \cdot |\zeta_1^k \zeta_2^l (\mathcal{F}\chi)^\mathbb{C}| \leq c_{0,0} c_{k,l} \exp(2b_1|\mathrm{Im}\zeta_1| + 2b_2|\mathrm{Im}\zeta_2|)$, so that $g \in \mathcal{Z}(\mathbb{C}^2)$.

Note that the condition (2.36) is more restrictive than the positivity condition (2.29), because functions $\langle\alpha|\psi\rangle$ are of a very specific form: for any $|\psi\rangle \in L^2(\mathbb{R})$, $\langle\alpha|\psi\rangle = \mathrm{e}^{-|\alpha|^2/2} f_\psi(\overline{\alpha})$, where $f_\psi(\overline{\alpha})$ is an entire function — the, so called, Fock-Bargmann representation of the vector $|\psi\rangle$ (see e.g. Perelomov [72], Klauder and Sudarshan [47], or Carlen [11] for more information).

The equivalent form of Theorem 2.3 is that a state ϱ is genuine quantum if and only if there exists a test function $f \in \mathcal{Z}(\mathbb{C}^2)$, such that: $\int \mathrm{d}^2\alpha\, P_\varrho(\alpha, \overline{\alpha})\, |f_\mathbb{R}(\alpha, \overline{\alpha})|^2 < 0$. Since by its definition $f_\mathbb{R}$ is real-analytic in $\mathrm{Re}\alpha$ and $\mathrm{Im}\alpha$, the latter condition can be rewritten in the operator form:

$$\mathrm{tr}\big(\varrho : |f_\mathbb{R}(a, a^\dagger)|^2 : \big) < 0\,, \tag{2.37}$$

implying that the state is nonclassical if and only if there exists an observable $: |f_\mathbb{R}(a, a^\dagger)|^2 :$ detecting it.

Geometrically, the condition $\int \mathrm{d}^2\alpha\, P_\varrho(\alpha, \overline{\alpha})\, |f_\mathbb{R}(\alpha, \overline{\alpha})|^2 = 0$ defines a hyperplane in the set of all P-distributions and hence a state is nonclassical if and only if there is a hyperplane separating it from the simplex of classical states Δ. This is a special case of the powerful Hahn-Banach Theorem and, from the physical point of view, essentially the same approach as the one used in the method of the, so called, entanglement witnesses. We will introduce this method in Section 3.1 of Chapter 3 and then use in Chapter 5. Motivated by this analogy, we call the observables from the expression (2.37) *non-classicality witnesses*. Then, the condition (2.36) provides the complete family of witnesses, describing the simplex of classical states Δ.

The above approach can be generalized if one allows the test functions f to depend on the state ϱ in question. Then, observables in the inequality (2.37) becomes non-linear functions of the state, and may be termed a *non-linear non-classicality witnesses* (similar non-linear witnesses were also used in the study of entanglement, e.g. in the work of Gühne [33]).

2.4 Connection to Hilbert's 17th problem

2.4.1 States with smooth $\mathcal{F}P_\varrho$

Theorem 2.3 from the previous Section is general and applies to any density matrix on $L^2(\mathbb{R})$. The price to pay for this generality is that the space of the test functions is rather complicated. On the other hand, one would like to be able to use in the criterion (2.37) some simple witnesses, like, for example, those polynomially depending on the annihilation and creation operators a and $a^\dagger$. Such witnesses can be in principle experimentally implemented, which we discuss briefly in Section 2.5.

Thus, it is an interesting task to examine under which circumstances they can be used.

Unfortunately, for a general state ϱ, the action of P_ϱ is not well defined on polynomials in the real parameters[3] $x := \mathrm{Re}\alpha$ and $y := \mathrm{Im}\alpha$. This follows from the following argument. Denote the space of all complex polynomials in (x, y) by $\mathbb{C}[x, y]$. From the basic properties of the distributional Fourier transform, every $w \in \mathbb{C}[x, y]$ is a Fourier transforms of a distribution T_w of the form:

$$T_w(x, y) = \sum_{ij} t(w)_{ij} \frac{\partial^{i+j}}{\partial x^i y^j} \delta^2(x, y)\,. \tag{2.38}$$

Suppose that the action of P_ϱ can be defined on polynomials. Then from the definition (2.23) it would follow that:

$$\langle P_\varrho, \mathcal{F}T_w\rangle = \langle \mathcal{F}P_\varrho, T_w\rangle, \tag{2.39}$$

but the right hand side of the above equation generically may not be well defined — we were able to prove only the continuity of $\mathcal{F}P_\varrho$ through Eq. (2.20), but not its differentiability.

Hence, in order to be able to use in the criterion (2.37) with arbitrary polynomial witnesses, it is sufficient to narrow down the space of states in question to those ϱ's, for which $\mathcal{F}P_\varrho$'s are smooth functions on $\mathbb{R}^2$. Then, the action of P_ϱ on polynomials is well defined through Eqs. (2.38) and (2.39). Apparently, this space, denoted by $S^\infty(\mathbb{R})$, is quite large and contains most of the physically relevant families of states, e.g. Fock and Gaussian states.

Let us now examine how general Theorem 2.3 looks like for $\varrho \in S^\infty(\mathbb{R})$. Let f be an arbitrary function from $\mathcal{Z}(\mathbb{C}^2)$. Since f is entire, we have that:

$$f(\zeta_1, \zeta_2) = \sum_{n_1, n_2} c_{n_1, n_2} (\zeta_1 - a)^{n_1} (\zeta_2 - b)^{n_2} \tag{2.40}$$

for an arbitrary $(a, b) \in \mathbb{C}^2$, and the series converges almost uniformly, i.e. uniformly on each compact subset, and absolutely on $\mathbb{C}^2$. Hence, there exists a double sequence $\{w_n\}_{n=(n_1,n_2)}$ of polynomials from $\mathbb{C}[\zeta_1, \zeta_2]$ — the partial sums of the double series from Eq. (2.40), such that: $w_n \underset{a.u.}{\longrightarrow} f$, where $\underset{a.u.}{\longrightarrow}$ denotes the almost uniform convergence. By taking the real and imaginary parts of w_n and restricting them to $\mathbb{R}^2$ (by setting the imaginary parts of (ζ_1, ζ_2) to zero), we obtain that there exists a pair of sequences $\{u_n, v_n\}$ of real polynomials from $\mathbb{R}[x, y]$, $x = \mathrm{Re}\zeta_1$, $y = \mathrm{Re}\zeta_2$, such that: $u_n \underset{a.u.}{\longrightarrow} \mathrm{Re}f_\mathbb{R}$ and $v_n \underset{a.u.}{\longrightarrow} \mathrm{Im}f_\mathbb{R}$. As $u_n(x, y)$ it is enough to take $\mathrm{Re}\, w_n(x, y)$, while as $v_n(x, y)$, $\mathrm{Im}\, w_n(x, y)$. Since the convergence in Eq. (2.40) is absolute, we also obtain that:

$$u_n^2 + v_n^2 \underset{a.u.}{\longrightarrow} |f_\mathbb{R}|^2. \tag{2.41}$$

[3]It is more convenient to use this parameters here instead of the phase-space related ones (ξ, η) defined in Eq. (2.6).

But the almost uniform convergence on the real plane, as it appears in Eq. (2.41), defines the convergence in $\mathcal{Z}(\mathbb{C}^2)$, as we indicated in the previous Section. Thus, after substituting the approximation (2.41), valid for any $f \in \mathcal{Z}(\mathbb{C}^2)$, into the integral in the condition (2.36), we can interchange the integration and taking the limit:

$$\int P_\varrho \, |f_{\mathbb{R}}|^2 = \lim_{n\to\infty} \int P_\varrho \, (u_n^2 + v_n^2) \, . \tag{2.42}$$

This leads us to the main result of the developed approach:

Theorem 2.4. *A state $\varrho \in S^\infty(\mathbb{R})$ is classical if and only if:*

$$\int d^2\alpha \, P_\varrho(\alpha, \overline{\alpha}) \, v(\alpha, \overline{\alpha})^2 = \mathrm{tr}[\varrho : \mathrm{v}(\mathrm{a}, \mathrm{a}^\dagger)^2 :] \geq 0 \tag{2.43}$$

for every real polynomial $v \in \mathbb{R}[x, y]$.

In fact, at least two particular cases of the criterion (2.43) has already been wildly used in quantum optics and are standard tools for detecting important classes of genuine quantum states. One of such standard non-classicality tests is the test for higher order quadrature squeezing, introduced by Hong and Mandel in Ref. [38]:

Definition 2.4. *A state ϱ is called squeezed to the order $2k$ if there exists a phase $\varphi \in [0, 2\pi)$ such that:*

$$\sum_{l=0}^{k-1} \frac{1}{2^l} \frac{(2k)!}{l![2(k-l)]!} \langle : (\Delta E_\varphi)^{2(k-l)} : \rangle < 0 \, , \tag{2.44}$$

where $E_\varphi := a e^{-i\varphi} + a^\dagger e^{i\varphi}$, $\Delta E_\varphi := E_\varphi - \langle E_\varphi \rangle$, and all the averages are taken with respect to ϱ.

Obviously, the inequality (2.44) has the form of a violation of the condition (2.43) (we can always substitute v^2 there with finite sums of such terms) with the specific polynomial:

$$w_{2k}(x, y; \varphi) := \sum_{l=0}^{k-1} \frac{1}{2^l} \frac{(2k)!}{l![2(k-l)]!} [d_\varphi(x, y)]^{2(k-l)} \, , \tag{2.45}$$

where:

$$d_\varphi(x, y) := 2 \left[x - \left\langle \frac{a + a^\dagger}{2} \right\rangle \right] \cos\varphi + 2 \left[y - \left\langle \frac{a - a^\dagger}{2\mathrm{i}} \right\rangle \right] \sin\varphi \, . \tag{2.46}$$

The witness w_{2k} depends on the tested state ϱ and hence it is a nonlinear witness, according to the terminology of the previous Section.

The second special case of Theorem 2.4 is the test for sub-Poissonian statistics of $a^\dagger a$, also known as number squeezing:

Definition 2.5. *A state ϱ is called number squeezed if $\langle : (\Delta a^\dagger a)^2 : \rangle < 0$.*

The corresponding nonlinear witness reads:

$$w_P(x,y) := (x^2 + y^2 - \langle a^\dagger a \rangle)^2 \,. \tag{2.47}$$

In this sense the criterion (2.43) generalizes the standard notions of squeezing in quantum optics. Note also that both nonlinear witnesses (2.45) and (2.47) are optimal in the sense that they are zero on the extreme points of Δ, i.e. on the pure coherent states $|\alpha\rangle\langle\alpha|$, since from Eq. (2.4) it follows that for any coherent state $|\alpha\rangle$, all the moments of normally ordered deviations vanish.

2.4.2 Hilbert's 17th problem and polynomial witnesses

Closer examination of Theorem 2.4 reveals an interesting connection of the problem of quantumness of states from $S^\infty(\mathbb{R})$ to one of a basic problems in real algebra. It is a trivial observation that for any real polynomial in n variables $v \in \mathbb{R}[x_1, \ldots, x_n]$, its square v^2 is positive semidefinite (*PSD*). The same is automatically true for every polynomial $p \in \mathbb{R}[x_1, \ldots, x_n]$ which is a finite sum of such terms: $p = \sum_k (v_k)^2$. Such polynomials are called *SOS* (Sum-Of-Squares) polynomials. Let us denote the space of homogeneous PSD polynomials of an even degree m in n variables by $P_{n,m}$, and the space of the corresponding SOS polynomials by $\Sigma_{n,m}$. Thus, we obviously have that $\Sigma_{n,m} \subset P_{n,m}$ for any n, m. One may ask if the converse is also true, i.e. if $\Sigma_{n,m} = P_{n,m}$, so that every PSD polynomial is SOS?

This problem has been known in mathematics under the name of Hilbert's 17th problem. The answer is, quite surprisingly, negative: there are PSD polynomials which are not SOS. This fact was proven by Hilbert in 1888. He showed that the equality $\Sigma_{n,m} = P_{n,m}$ holds only for $n \leq 2$ or $m \leq 2$, or $n = 3$ and $m = 4$. However, Hilbert's proof was not constructive and the explicit examples of PSD but not SOS polynomials are rare and started to appear only in the 1960's.

After proving that generically $\Sigma_{n,m} \neq P_{n,m}$ Hilbert posed a more general question: is any PSD polynomial sum of squares of rational functions? This was actually the question number 17 in his famous lecture, delivered to the International Congress of Mathematicians in Paris in 1900. Such posed question was affirmatively answered by E. Artin in 1926. We refer the reader to the survey article of Reznick [77] for further information on the history and the present status of Hilbert's 17th problem.

In light of Theorem 2.4, out of all PSD polynomials, SOS polynomials are sufficient to detect nonclassical states among the states from $S^\infty(\mathbb{R})$. To illustrate how Theorem 2.4 works, let us consider a specific example of sixth order Motzkin polynomial M, which is PSD but non-SOS:

$$M(x,y,z) := (x^2 + y^2 - 3z^2)x^2y^2 + z^6 \,. \tag{2.48}$$

Using a method originating from the witness techniques in entanglement study (see Lewenstein *et al.* [61]), we construct an example of state ϱ_M, detected by the polynomial $M(x,y,\pm 1)$. Note that the polynomial (2.48) is homogeneous and depends on three variables, unlike the polynomials appearing in the criterion (2.43). But

any homogeneous polynomial from $\mathbb{R}[x,y,z]$ can be dehomogenized by setting $z=1$ and vice versa: by introducing a third variable z, any generic $v \in \mathbb{R}[x,y]$ can be homogenized. The property of being PSD or SOS is conserved under de- and homogenization.

The construction of ϱ_M goes as follows. Out of the four zeros $\{(\pm 1, \pm 1)\}$ of $M(x,y,\pm 1)$ we first construct four coherent states: $\alpha_1 := 1+\mathrm{i}$, $\alpha_2 := -1+\mathrm{i}$, $\alpha_3 := \overline{\alpha_2}$, and $\alpha_4 := \overline{\alpha_1}$. We then pick the barycentric point, $\tilde{\varrho}$, of the face $\mathcal{F} := \mathrm{conv}\{\delta(\alpha-\alpha_1),\ldots,\delta(\alpha-\alpha_4)\}$ (conv stands for a convex hull) of Δ spanned by them. The hyperplane defined by the witness $:M(a,a^\dagger,\pm 1):$

$$h_M := \{\varrho \in S^\infty(\mathbb{R}); \int \mathrm{d}x\,\mathrm{d}y\, P_\varrho(x,y) M(x,y,\pm 1) = 0\}\,, \tag{2.49}$$

contains the face $\mathcal{F} \subset \Delta$ and hence the witness is optimal. Thus, to get the state detected by the polynomial (2.48), we mix $\tilde{\varrho}$ with a projector onto an arbitrary vector from its range:

$$\varrho_M := (1-\epsilon)\tilde{\varrho} + \epsilon |\psi_M\rangle\langle\psi_M| = \frac{1-\epsilon}{4}\sum_{j=1}^{4} |\alpha_j\rangle\langle\alpha_j| + \epsilon |\psi_M\rangle\langle\psi_M|\,, \tag{2.50}$$

which for simplicity we choose to be:

$$|\psi_M\rangle := \frac{1}{N}(|\alpha_i\rangle + |\overline{\alpha_i}\rangle)\,, \quad N^2 := 2[1+\mathrm{e}^{-2}\cos(2)]\,. \tag{2.51}$$

Here $0 \le \epsilon \le 1$ and $i \in \{1,2,3,4\}$ is fixed, but the results presented below do not depend on its particular value. Calculating the average of the polynomial (2.48) using the expression (2.43), we obtain that:

$$\langle :M(a,a^\dagger,\pm 1):\rangle = (2/N^2)\,\mathrm{e}^{-2}\cos(2)\,\epsilon. \tag{2.52}$$

Since $\cos(2) < 0$, the state (2.50) is detected by M for $\epsilon > 0$.

As a side remark, note that the state (2.50) is also detected by another example of PSD, but non-SOS polynomial - Choi-Lam polynomial:

$$S(x,y,z) := x^4y^2 + y^4z^2 + z^4x^2 - 3x^2y^2z^2, \tag{2.53}$$

since $\langle :S(a,a^\dagger,\pm 1):\rangle_{\varrho_M} = -(4/N^2)\mathrm{e}^{-2}\sin(2)\,\epsilon < 0\,.$

However, we know from Theorem 2.4 that there must be a SOS polynomial detecting ϱ_M. Before we explicitly construct it, let us first examine the physically relevant witnesses (2.45) and (2.47). A simple calculation gives:

$$\begin{aligned}\langle :(\Delta a^\dagger a)^2: \rangle &= 4\Big[1 - 4\epsilon\frac{\mathrm{e}^{-2}\cos(2)}{N^2}\Big] \\ &- 4\left\{1 - 2\epsilon\frac{\mathrm{e}^{-2}[\sin(2)+\cos(2)]}{N^2}\right\}^2,\end{aligned} \tag{2.54}$$

which is non-negative for any $0 < \epsilon \le 1$. Examination of the witnesses w_{2k} from Eq. (2.45) is more difficult and we have carried it out only numerically. We checked

that up to the 14th order ($k = 7$) all the inequalities (2.44) are violated for any $\varphi \in [0, 2\pi)$ and $0 < \epsilon \leq 1$ and hence the state (2.50) is not squeezed up to the order of 14. Apart from that, we used a modified version of w_4, namely $\widetilde{w}_4 := d_{\varphi_1}(x,y)^2 d_{\varphi_2}(x,y)^2 + 6 d_{\varphi_3}(x,y)^2$, depending on three angles φ_1, φ_2 and φ_3, also with no success. The question if ϱ_M has even higher order squeezing is open.

To construct a SOS polynomial detecting ϱ_M, note that $M(x, y, \pm 1)$ has only four zeros, and hence we can find a second order polynomial with the same zeros, which squared will give us the desired witness. Equivalently, we look for such a SOS witness W that its hyperplane h_W, defined as in Eq. (2.49), contains the face $\mathcal{F}$. We choose $W(x,y) = (Ax^2 + By^2 + Cxy + Dx + Ey + F)^2$. The condition $W(\pm 1, \pm 1) = 0$ leads to a system of four linear equations for the coefficients $A, \ldots, F$. Its solution gives a family of witnesses $W_{A,B}(x,y) = (Ax^2 + By^2 - A - B)^2$, where $A^2 + B^2 \neq 0$. The average of $W_{A,B}$ in the state (2.50) is negative if and only if

$$\cos(2)\left[(A+B)^2 - 4A^2\right] + 4\sin(2)A[A+B] < 0. \tag{2.55}$$

As this equation possesses non-zero solutions, for example $A = 0, B \neq 0$, the state ϱ_M can be detected by a fourth order SOS polynomial.

This seems to be a generic feature, at least for the PSD polynomials of degree $m = 6$. In this case it is known (Reznick [77]) that if a PSD polynomial has exactly ten zeros in the projective space $\mathbb{R}P^3$, than it cannot be SOS. Fixing the variable z generally reduced the amount of zeros and hence permits to find a lower order SOS polynomial with the same zeros.

2.4.3 Hierarchy of classical states

The methods described above, together with Theorem 2.4, can be used to classify the classical states from $S^\infty(\mathbb{R})$, according to the degree of a SOS polynomial detecting them. Let us define a family of convex subsets of $S^\infty(\mathbb{R})$ by:

$$S_m := \bigcap_{w \in \widetilde{\Sigma}_{2,m}} \{\varrho \in S^\infty(\mathbb{R}); \int \mathrm{d}^2\alpha \, P_\varrho \, w \geq 0\}, \tag{2.56}$$

where $\widetilde{\Sigma}_{2,m}$ is the set of inhomogeneous SOS polynomials of degree m in (x, y). Theorem 2.4 implies that $\Delta = \bigcap_k S_{2k}$. It is also clear that $\widetilde{\Sigma}_2 \subset \widetilde{\Sigma}_4 \subset \cdots$ and hence $S_2 \supset S_4 \supset \cdots$. We prove a stronger result:

Theorem 2.5. *$S_2 \supsetneq S_4 \supsetneq \cdots$, i.e. for any even m there exists a nonclassical state detected by some witness from $\widetilde{\Sigma}_m$, and not detected by any witness from $\widetilde{\Sigma}_{(m-2)}$.*

Proof. Let us choose a generic SOS polynomial $w \in \widetilde{\Sigma}_m$. It has $(m+1)(m+2)/2$ terms, as it is a sum of polynomials of degree $\leq m$. From the variety $V(w) := \{(x,y); w(x,y) = 0\}$ we pick n points $(x_1, y_1), \ldots, (x_n, y_n)$, where $m(m+1)/2 < n < (m+1)(m+2)/2$, such that they do not lie on any variety of the form $V(u)$, where $u \in \widetilde{\Sigma}_{(m-2)}$. We can find such points, as otherwise there would exist a SOS

polynomial $u \in \widetilde{\Sigma}_{(m-2)}$, such that $(x_1, y_1), \ldots, (x_n, y_n) \in V(u)$. However, with the chosen number of zeros of w, n, the latter condition leads to an overcomplete system of linear homogeneous equations for the coefficients of u, which generically possesses no solution. On the other hand, the same condition for $V(w)$ yields a under-determined system possessing a non-trivial solution. Having such points, we construct coherent states $|x_1 + \mathrm{i}y_1\rangle, \ldots, |x_n + \mathrm{i}y_n\rangle$ and a face $\mathcal{F}_n \in \Delta$ spanned by them, just like we did when we were constructing the state ϱ_M. For any $\widetilde{\varrho} \in \mathcal{F}_n$ (for example the barycentric point) we have then that $\mathrm{tr}[\widetilde{\varrho}\, :w(a, a^\dagger):] = 0$, whereas $\mathrm{tr}[\widetilde{\varrho}\, :u(a, a^\dagger):] > 0$ for all SOS polynomials $u \in \widetilde{\Sigma}_{(m-2)}$. Hence, from the continuity of the expectation value $\mathrm{tr}[\varrho A]$ with respect to ϱ, we can find a convex combination ϱ_w of $\widetilde{\varrho}$ and a projector onto some linear combination of $|x_1 + \mathrm{i}y_1\rangle, \ldots, |x_n + \mathrm{i}y_n\rangle$, such that $\mathrm{tr}[\varrho_w\, :w(a, a^\dagger):] < 0$, while for all $u \in \widetilde{\Sigma}_{(m-2)}$, $\mathrm{tr}[\varrho_w\, :u(a, a^\dagger):] \geq 0$. □

2.5 Discussion

First of all, let us note that the generalization to n-dimensional systems, like n-mode electromagnetic fields, is rather straightforward. The analog of Theorem 2.1 from Section 2.2 states that any state ϱ can be uniquely decomposed into the projectors $|\alpha_1, \ldots, \alpha_n\rangle\langle\alpha_1, \ldots, \alpha_n|$ with P_ϱ now being an ultradistribution from $\mathcal{Z}(\mathbb{R}^{2n})$. Then the test functions f in Theorem 2.3 are from the space $\mathcal{Z}(\mathbb{C}^{2n})$ and, correspondingly, the space of the test polynomials in Theorem 2.4 becomes $\mathbb{R}[x_1, \ldots, x_n, y_1, \ldots, y_n]$.

Next, note that although we were implicitly analyzing states of a harmonic oscillator, we can also apply all the preceding analysis to *any* mechanical system. As we stressed in Section 2.2, coherent states can be defined independently of the dynamics of the system under consideration, as the states minimizing the uncertainty relations. Then, the Fock vacuum $|0\rangle$ is defined as the unique state with the vanishing expectation values of position and momentum[4]. We can then argue that Eq. (2.6) still provides a valid way of embedding the classical phase-space in the quantum Hilbert space and use the same definition of classicality 2.1. However, since coherent states are preserved only by Hamiltonians at most quadratic in position and momentum, classicality or genuine quantumness will becomes a dynamical property.

Finally, let us discuss experimental consequences of the proposed method. Polynomial *non-classicality witnesses* can be in principle easily measured, allowing thus for a direct detection of quantumness and its degree for a given state. In this sense they are similar to *entanglement witnesses*, which we define in the next Chapter, that are nowadays commonly used for detection of entanglement (see e.g. Barbieri *et al.* [4], Eibl *et al.* [21]). If one wants to check if a given state ϱ is quantum, it is enough to measure normally ordered averages of squares of real polynomials of $\hat{q}$ and $\hat{p}$, or quadrature operators. In order to check the degree of quantumness (i.e. to check whether $\varrho \in S_{2k}$), one should determine normally ordered averages of squares of real polynomials of the order k. Note that for a given k this requires

[4]More generally, one can define coherent states by an analog of Eq. (2.6): $|\alpha\rangle := W(\alpha)|\psi_0\rangle$, where $|\psi_0\rangle$ is an arbitrary vector, not necessarily the Fock vacuum; see Perelomov [72] for the general theory of coherent states.

measurements of finite number of averages only. For instance, for $k = 1$ (squeezing), one needs to measure $\langle \hat{q} \rangle$, $\langle \hat{p} \rangle$, $\langle :\hat{q}^2: \rangle$, $\langle :\hat{p}^2: \rangle$, and $\langle :\hat{q}\hat{p} + \hat{p}\hat{q}: \rangle$, and check if there exist A, B, C such that $\langle :(A\hat{q} + B\hat{p} + C)^2: \rangle < 0$. For a general k, one needs respectively $k(2k + 3)$ measurements.

Chapter 3

Group-theoretical approach to entanglement

In this Chapter we introduce the notion of quantum entanglement and briefly discuss the associated separability problem. Then, we present a novel, universal description of quantum entanglement using group theory and generalized characteristic functions. It leads to new reformulations of the separability problem, and the positivity of partial transpose (PPT) criterion. Application of our method to finite groups leads to an embedding of the separability problem in a given dimension into a higher dimensional one, but with a high symmetry. Within the group-theoretical formalism, we also show a connection between the existence of entanglement and group non-commutativity.

3.1 Entanglement and the separability problem

3.1.1 Definitions and historical remarks

In this Chapter we study another aspect of quantumness, associated with multipartite systems. According to the basic axioms of quantum mechanics, if a system S_1 is described by a Hilbert space $\mathcal{H}_1$, system S_2 by $\mathcal{H}_2$, then the composite system S_{12} is described by the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$. The latter space can be spanned by *product vectors*, i.e. by vectors $|\psi\rangle$, which can be represented as:

$$|\psi\rangle = |u\rangle \otimes |v\rangle, \tag{3.1}$$

where $|u\rangle \in \mathcal{H}_1$ and $|v\rangle \in \mathcal{H}_2$.

Physical meaning of product vectors is rather easy to understand: they represent those states of the composite system, in which the subsystems are statistically independent. That is, if the system is in a product state (3.1) and one measures some observable $A = \sum_\mu a_\mu P_\mu$ on the system S_1 and some observable $B = \sum_\nu b_\nu Q_\nu$ on the system S_2 (the sums are the corresponding spectral decompositions), then

the probability $p_\psi(\mu,\nu|A,B)$ of obtaining the value a_μ for A and b_ν for B is given by:

$$p_\psi(\mu,\nu|A,B) := \langle\psi|P_\mu \otimes Q_\nu\psi\rangle = p_u(\mu|A)\, p_v(\nu|B) \tag{3.2}$$

according to the classical law of the joint probability of independent events. However, due to the linear superposition principle, one has to allow also for the linear combinations of product states, which generically are not product. This leads to:

Definition 3.1. *A vector $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is called entangled if it cannot be represented in the form (3.1), i.e. if it is not product.*

Unlike product vectors, entangled vectors, or pure entangled states in other words, imply rather peculiar properties of quantum mechanics and, in our opinion, their role is yet to be fully understood. The first account of such a peculiar property was made by Einstein, Podolsky and Rosen in their seminal work [22] from 1935. The authors argued that the if one accepts that quantities predictable with probability one correspond to "elements of reality" and that the wave functions contain the complete information about mechanical systems, then one reaches a contradiction. They considered a bipartite system described by a certain pure entangled state and showed that then one can assign to each subsystem with certainty simultaneous values of position and momentum. This analysis led Einstein to speak about the "spooky action at a distance" in quantum mechanics.

The philosophical rather than physical work of Einstein, Podolsky and Rosen was brought to actually experimentally accessible level by Bell in 1964 (Bell's works are collected in Bell [5]). Bell essentially showed that statistical properties of a system in a pure entangled state cannot be simulated by a local classical probability distribution, i.e. it is not possible to construct a local hidden variables (LHV) model, reproducing the predictions of quantum mechanics. Usually, and in our eyes without a firm ground, this property is interpreted as "non-locality" of quantum mechanics. Let us however state it clearly that no superluminal signalling is possible within the present quantum theory. Bell's statement is formulated in a form of the famous inequalities, named after Bell himself, which are satisfied only within LHV models[1]. In the recent years there have been performed various experimental tests of Bell inequalities (see e.g. Rowe *et al.* [82]), suggesting that they are indeed violated in Nature. However, all of those experiments contain open loopholes (two major being the, so called, locality and efficiency loopholes), and hence the violation of Bell inequalities is still not unambiguously experimentally demonstrated.

So far we have been considering only pure states. The generalization of the notion of entanglement to arbitrary mixed states was proposed by Werner [102] in 1989. Werner considered the following scenario: experimentalists in two separate laboratories share two individual systems S_1 and S_2. They prepare their systems in one of the states (without loss of generality we may assume pure): $|u_1\rangle,\ldots,|u_K\rangle$ and $|v_1\rangle,\ldots,|v_K\rangle$ respectively, according to a common random number generator,

[1] Werner and Wolf [104] contains an excellent survey on LHV models, Bell inequalities, and related topics.

correlating their actions. The resulting state of the composite system is then:

$$\varrho = \sum_{i=1}^{K} p_i |u_i\rangle\langle u_i| \otimes |v_i\rangle\langle v_i|, \tag{3.3}$$

where p_i are the probabilities describing the random number generator and satisfying $\sum_i p_i = 1$. This leads us to the following:

Definition 3.2. *A state ϱ of a composite system is called separable, or classically correlated, if it can be represented as a norm limit of the states of the type (3.3). Otherwise it is called entangled.*

Thus, a state is separable if it can be represented as a convex decomposition of pure product states. This definition leads to a natural question, known as the *separability problem*: given a state ϱ decide weather it is separable or not.

Despite numerous attempts (we name some of them in the next Subsection; see also e.g. Lewenstein *et al.* [62]) and substantial time passed after its formulation, the efficient (given finite computational resources) algorithm of answering the above question in generic dimension is still not known.

To emphasize its importance, let us mention that apart from the "spooky action at a distance" and the "quantum non-locality", the study of entangled states led to the discovery that apart from classical information, there exists also quantum information (although there is no precise definition yet). Just like its classical counterpart, quantum information can be processed and stored. Practical applications include quantum teleportation, dense coding, and cryptography to name a few. We refer to e.g. Peres [73], Nielsen and Chuang [70], and Bouwmester *et al.* [8] for a detailed account of of the quantum information theory and the related topics. Also, there are attempts to incorporate quantum information into the very foundations of quantum mechanics (see e.g. Rovelli [81], Horodecki *et al.* [41] and Clifton *et al.* [13]). Thus, the ability of efficient distinguishing between separable and entangled states is of both fundamental and practical importance.

3.1.2 Some known facts about the separability problem

In the case of the pure states distinguishing between product and entangled vectors is rather easy and there is a number of necessary and sufficient conditions available. One of them (and historically the oldest) is based on the, so called, Schmidt decomposition (see e.g. Peres [73]). The other one, which we shall use in the sequel, is given by the following Proposition:

Proposition 3.1. *A vector $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is product if and only if*

$$\mathrm{tr}_1(\mathrm{tr}_2|\psi\rangle\langle\psi|)^2 = ||\psi||^4 = \mathrm{tr}_2(\mathrm{tr}_1|\psi\rangle\langle\psi|)^2. \tag{3.4}$$

For general mixed states the situation is much more complicated and a few introductory remarks are in order. Let us denote the space of all separable states by

Sep. Then it is a convex subset of the set of all states — the convex hull of the set of all pure product states, constituting the extreme points of *Sep*. Since *Sep* is by definition also closed, the separability problem, just like the quantumness problem of Chapter 2, is a special case of the, so called, convex membership problem: given a point in some vector space X decide if it belongs to a given closed convex subset of X.

In principle, there exist at least two formal solutions to the separability problem. The first one, and the most general one, valid in any dimension, is provided by the Hahn-Banach Theorem (see e.g. Rudin [83]), which states that a point in a locally convex vector space X can always be separated by a hyperplane from any closed convex subset of X. We have already encountered an example of such situation when studying the quantumness of states in the previous Chapter (see the last paragraph of Section 2.3 and Eq. (2.49)). In case of the separability problem, the underlying space X is the space of all trace-class operators on $\mathcal{H}_1 \otimes \mathcal{H}_2$. Since it carries an additional structure of a Hilbert space with respect to the Hilbert-Schmidt scalar product, some simplifications occur. First of all, let us define:

Definition 3.3. *An entanglement witness is a hermitean operator $\mathcal{W}$, such that* $\mathrm{tr}(\mathcal{W}\varrho) \geq 0$ *for all separable states and there exists an entangled state $\varrho_{\mathcal{W}}$ such that* $\mathrm{tr}(\mathcal{W}\varrho_{\mathcal{W}}) < 0$. *Then it is said that $\mathcal{W}$ detects the state $\varrho_{\mathcal{W}}$.*

Then, each witness $\mathcal{W}$ defines a separating hyperplane $h_{\mathcal{W}}$ by the equation $\mathrm{tr}(\mathcal{W}A) = 0$. Thanks to the Riesz Lemma, Hahn-Banach Theorem can be reformulated in a form of an entanglement test (Horodecki *et al.* [39], Terhal [97]):

Theorem 3.1. *A state ϱ is entangled if and only if there exists an entanglement witness $\mathcal{W}_\varrho$ detecting it.*

Unfortunately, the proof of the Hahn-Banach Theorem is non-constructive and thus does not provide a prescription for finding entanglement witnesses. However, Terhal [97] and Lewenstein *et al.* [61] introduced and developed a method, known as the method of *entanglement witnesses*, for doing so, provided we know which state (or family of states) we want to detect. This is in contrast with the situation we dealt with in the previous Chapter. There we were able to identify *all* possible non-classicality witnesses: for states from $S^\infty(\mathbb{R})$ they were given by all SOS polynomials (c.f. Theorem 2.4). The method of entanglement witnesses will be further used in Chapter 5.

Another, more elaborate, reformulation of the Hahn-Banach Theorem, connects the separability problem with one of the open problems in functional analysis (Horodecki *et al.* [39]):

Theorem 3.2 (M. Horodecki, P. Horodecki, R. Horodecki). *A state ϱ is separable if and only if for every positive, linear map $\Lambda\colon B(\mathcal{H}_1) \to B(\mathcal{H}_2)$ it holds:* $(\Lambda \otimes \mathbf{1})\varrho \geq 0$.

A map Λ is called positive if for every operator $A \geq 0$, $\Lambda(A) \geq 0$. If moreover for every extension $\Lambda \otimes \mathbf{1}$ the resulting map is also positive, then Λ is called *completely*

positive or a CP-map[2] . Theorem 3.2 provides thus the characterization of separable states in terms of maps which are positive but not completely positive. Although the parametrization of CP-maps is known and is given by the, so called, Kraus decomposition (Kraus [55]), the characterization of positive but not completely positive maps is still unknown (apart from some special examples; see Størmer [95] and Woronowicz [110]).

Before we describe the second formal solution of the separability problem, let us specify to the case of systems described by finite dimensional Hilbert spaces (like spin systems). Throughout this work we study separability problem only for such systems. Thus, without a loss of generality, we may assume that $\mathcal{H}_1 = \mathbb{C}^m$ and $\mathcal{H}_2 = \mathbb{C}^n$. Then, the set of all states, and hence the set of all separable states, is a convex compact subset of $\mathbb{R}^{m^2n^2-1}$. Actually, in finite dimension we may drop the norm closure from Definition 3.2, as then the set of all pure product states is compact (it is diffeomorphic to $\mathbb{C}P^m \times \mathbb{C}P^n$), and hence its convex hull Sep is compact too. Moreover, the following fact holds:

Theorem 3.3 (Caratheodory). *Each point of a convex subset S of $\mathbb{R}^k$ can be represented as a convex combination of no more than $k+1$ affinely independent extreme points of S.*

Hence, every element of Sep can be decomposed into at most m^2n^2 product states. However, unlike in the classical case (Mielnik [66]), the decomposition of a given quantum state ϱ into a convex mixture of pure states is highly non-unique, which makes the separability problem so difficult to solve. We describe this non-uniqueness in more detail in Section 6.1.

The second formal solution of the separability problem comes then from the following observation: the separable decomposition (3.3), written in any product basis of $\mathbb{C}^m \otimes \mathbb{C}^n$, reads:

$$w_{\alpha\beta\mu\nu} := \sum_{i=1}^{K} p_i \, \overline{u_{i\alpha}} \, \overline{v_{i\beta}} \, u_{i\mu} v_{i\nu} - \varrho_{\alpha\beta\mu\nu} = 0. \tag{3.5}$$

Eq. (3.5) can be viewed as a system of real (after taking the real and imaginary parts) fourth order polynomial equations, imposed on the unknowns $\mathrm{Re}u_{i\alpha}$, $\mathrm{Im}u_{i\beta}$, $\mathrm{Re}v_{i\gamma}$, $\mathrm{Im}v_{i\gamma}$. Let us denote the set of solutions of the system (3.5) for a given ϱ by V_ϱ. Then the separability problem is equivalent to the question if V_ϱ is empty or not. The general solution is provided by the Real Nullstellensatz (see e.g. Bochnak *et al.* [7]), which says that $V_\varrho = \emptyset$ if and only if there exists a SOS polynomial s and polynomials $t_{\alpha\beta\mu\nu}$ such that:

$$-1 = s + \sum_{\alpha,\ldots,\nu} \mathrm{Re}\big(w_{\alpha\beta\mu\nu} \, \overline{t_{\alpha\beta\mu\nu}}\big). \tag{3.6}$$

However, finding such a certificate is computationally very difficult and inefficient , due to the fact that the degrees of s and $t_{\alpha\beta\mu\nu}$ are unbounded.

[2]Note that the proof of the Theorem 3.2 in one direction follows immediately from the definition of a separable state (3.3).

As we mentioned before, at the present day the efficient methods of solving the separability problem in generic dimension are still not known. We know only some partial results. One of the most important of them is the following necessary criterion of Peres [74]:

Theorem 3.4 (PPT). *If ϱ is separable then $\varrho^{T_1} \geq 0$ (or equivalently $\varrho^{T_2} \geq 0$), where the partial transposition is taken with respect to an arbitrary product basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$.*

Proof. Although the transposition itself is basis-dependent, the eigenvalues of the operator ϱ^{T_1} are basis-independent. Hence, we may work in an arbitrary basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$. Then, it easily follows from the very definition of a separable state (3.3) that for such a state: $\varrho^{T_1} = \sum p_i |u_i\rangle\langle u_i|^T \otimes |v_i\rangle\langle v_i| = \sum p_i |\overline{u_i}\rangle\langle\overline{u_i}| \otimes |v_i\rangle\langle v_i|$, where $|\overline{u_i}\rangle$ denotes the complex conjugation of the vector $|u_i\rangle$ in the basis where the transposition is calculated. But the last sum is a well defined state, and hence it is positive semidefinite. □

Apparently, this seemingly easy criterion gives both *necessary and sufficient* separability condition in the lowest dimensions $2 \otimes 2$ and $2 \otimes 3$, as it was proven by Horodecki *et al.* in Ref. [39]. The proof follows from the fact that in the lowest dimensions there exists a full characterization of positive but not completely positive maps, which implies that it is enough to consider only the transposition map in Theorem 3.2 (Woronowicz [110]). However, in higher dimensions there exist states with a positive partial transpose, which are nevertheless entangled (the, so called, *bound entangled* or PPT entangled states), as first shown by Horodecki in Ref. [40]. Nevertheless, this easy in implementation entanglement test is surprisingly powerful and remains one of the basic tools for probing entanglement.

The alternative to entanglement witnesses and PPT condition methods of detecting entangled states has been developed e.g. by Chen and Wu [12], Doherty *et al.* [18] (they present a very strong condition, detecting in principle almost all entangled states), Gühne [33], and the mentioned Horodecki [40]. It is also worth mentioning that a connection between Hilbert's 17th problem and the separability problem was established by Terhal in Ref. [98].

3.1.3 The outline of our approach

In this Chapter we present a novel, group-theoretical approach to the separability problem in finite dimension, introduced in our work [53]. It is closely linked to the methods of characteristic functions from the previous Chapter. Our method is based on a generalization of the notion of characteristic function and results from the following two observations: i) it is possible to identify a bipartite Hilbert space $\mathbb{C}^m \otimes \mathbb{C}^n$ with a tensor product of representation spaces of two irreducible, unitary representations of some compact group G; ii) one can then perform a non-commutative Fourier transform and assign to each density matrix a unique function on $G \times G$, satisfying certain positivity conditions. This function is an analog of a standard characteristic function of a probability distribution, introduced in Eq. (2.30) in the previous

Chapter, but is defined on a generically non-Abelian group. In the framework of non-commutative geometry, such functions are called *non-commutative characteristic functions* and we will use this term here also. The group G we call the *kinematical group* of an individual system. Although we do not present any new entanglement tests here, the results of this Chapter offer a new point of view on the separability problem, and link it to harmonic analysis and group theory.

3.2 Non-commutative characteristic functions

We begin with presenting the general set up. We consider an arbitrary compact group G (it may or may not be a Lie group) and let τ be any of its irreducible, unitary representation (in the sequel by representation we will always mean a unitary representation) acting in a Hilbert space $\mathcal{H}_\tau$. We study linear operators A acting in $\mathcal{H}_\tau$, and, in particular, density matrices ϱ. In the present Chapter we fix G to be compact and non-Abelian, as we consider here only finite dimensional systems, and for a compact group all of its irreducible unitary representations are necessarily finite dimensional (we will develop the formalism of non-commutative characteristic functions on a particular non-compact group in the next Chapter). Non-Abelian character of G also ensures that there are more than one-dimensional irreducible representations.

We assign to each operator A a continuous complex function ϕ_A on G through:

$$\phi_A(g) := \mathrm{tr}\big[A\tau(g)\big]\,. \tag{3.7}$$

For a particular case of a density matrix ϱ, the function ϕ_ϱ is a non-commutative analog of the usual Fourier transform of a probability measure, given by Eq. (2.30) — if we think of a state ϱ as of a quantum analog of a probability measure μ (see Mackey [63]), then ϕ_ϱ is an analog of its characteristic function $\mathcal{F}\mu$. Indeed, from the positivity of ϱ and Eq. (3.7), it follows that:

$$\iint_{G\times G} \mathrm{d}g\,\mathrm{d}h\overline{f(g)}\phi_\varrho(g^{-1}h)f(h) \geq 0 \text{ for any } f \in L^1(G), \tag{3.8}$$

where $\mathrm{d}g$ is the normalized Haar measure on G. Comparing the above condition with the definition of positive definiteness (Definition 2.3, Section 2.3), we see that the condition (3.8) is just a generalization of the latter to an arbitrary, not necessarily Abelian, group G [3]. Moreover, ϕ_ϱ is normalized, in the sense that:

$$\phi_\varrho(e) = 1 \tag{3.9}$$

(e denotes the neutral element of G), which follows from the normalization of ϱ. From the definition (2.30) the same holds for $\mathcal{F}\mu$: $\mathcal{F}\mu(0) = 1$. Thus, ϕ_ϱ possesses all

[3] Since ϕ is continuous, the condition (3.8) is also equivalent to an analog of the discrete condition from Theorem 2.2: ϕ is positive definite if for any N and any sequence $\{g_\alpha\} \in G$, $\alpha = 1, \ldots, N$ matrix $\phi(g_\alpha^{-1}g_\beta)$ is positive semidefinite.

the features of a classical characteristic function, but it is defined on a non-Abelian group.

This brings us to the connection between our approach and non-commutative geometry. In the framework of non-commutative geometry, density matrices, i.e. positive, normalized operators, are by definition the analogs of probabilistic measures on the corresponding quantum spaces. The map $A \mapsto \phi_A$ is viewed as the non-commutative generalization of the usual Fourier transform. Thus, from this point of view, functions ϕ_ϱ are exactly the characteristic functions of non-commutative measures. Hence the terminology — non-commutative characteristic functions.

Note that non-commutative characteristic functions (3.7) are generally easy to calculate explicitly. For example, when $G = SU(2)$ and $\tau = \tau_j$ carries spin j, they are polynomials of degree $2j$ in the group parameters. As an example, in Appendix A we calculate the characteristic function of the $3 \otimes 3$ PPT entangled Horodecki's state from Ref. [40].

The crucial point for our approach is that, since τ is irreducible, one can invert the non-commutative Fourier transform (3.7) and recover the operator A from its characteristic function:

$$A = \int_G \mathrm{d}g \; d_\tau \, \phi_A(g)\tau(g)^\dagger, \quad d_\tau := \dim \mathcal{H}_\tau. \tag{3.10}$$

The easy proof of (3.10) is obtained by taking the matrix elements of both sides in some orthonormal basis of $\mathcal{H}_\tau$, and then using the Peter-Weyl Theorem, which states, among the others that:

Theorem 3.5 (Peter-Weyl). *For any irreducible representation τ of a compact group G, holds:*

$$\int dg \, d_\tau \, \tau_{\mu\nu}(g)\overline{\tau_{\mu'\nu'}(g)} = \delta_{\mu\mu'}\delta_{\nu\nu'}, \tag{3.11}$$

where matrix elements $\tau_{\mu\nu} := \langle e_\mu | \tau e_\nu \rangle$ of τ are taken with respect to any orthonormal basis $\{|e_\mu\rangle\}$ of $\mathcal{H}_\tau$;

For any two non-equivalent irreducible representations π, τ of G their matrix elements are orthogonal: $\int dg \, \pi_{\mu\nu}(g)\overline{\tau_{\mu'\nu'}(g)} = 0$.

More details can be found in e.g. Folland [24] or Zhelobenko [112].

An interesting implication of Eq. (3.10) is that multiplication of operators corresponds to taking convolutions of the corresponding functions (3.7):

$$\phi_{AB} = d_\tau \phi_A * \phi_B, \tag{3.12}$$

where we defined the convolution product $*$ as follows:

$$f * f'(g) := \int_G \mathrm{d}h f(h) f'(gh^{-1}) = \int_G \mathrm{d}h f(h^{-1}g) f'(h) \tag{3.13}$$

(in the last step we substituted $h \to h^{-1}g$ and used the fact that $\mathrm{d}g^{-1} = \mathrm{d}g$ for compact groups; see Folland [24]). In particular, a state ϱ is pure if and only if:

$$\phi_\varrho = d_\tau \phi_\varrho * \phi_\varrho. \tag{3.14}$$

Let us now focus on the space of all normalized, positive definite functions on G, i. e. the space of all continuous functions ϕ, satisfying the conditions (3.8) and (3.9). We denote this space by $\mathcal{P}_1(G)$. It is a convex subset of the space of all continuous functions on G, and the set of its extreme points we denote by $\mathcal{E}_1(G)$. The structure of $\mathcal{E}_1(G)$ is described by the Gel'fand-Naimark-Segal (GNS) construction. Since we will need it in the next Chapter too, let us briefly recall it here, referring the reader to Folland [24] for more details:

Theorem 3.6 (Gel'fand-Naimark-Segal). *With each positive definite function ϕ on a locally compact group G one can uniquely, up to a unitary isomorphism, associate a triple $(\pi_\phi, \mathcal{H}_\phi, |\psi_\phi\rangle)$, where π_ϕ is a representation of G in a Hilbert space $\mathcal{H}_\phi$, $|\psi_\phi\rangle$ is a cyclic vector for this representation, i.e. the linear span of $\{\pi_\phi(g)|\psi_\phi\rangle\,;\, g \in G\}$ is dense in $\mathcal{H}_\phi$, and:*

$$\phi(g) = \langle \psi_\phi | \pi_\phi(g)\, \psi_\phi \rangle. \tag{3.15}$$

Generically, the representation π_ϕ is reducible and it is a deep result from the general theory of group representations that $\phi \in \mathcal{E}_1(G)$ if and only if the representation π_ϕ is irreducible. Thus, every $\phi \in \mathcal{E}_1(G)$ is a characteristic function of some pure state $|\psi_\phi\rangle \in \mathcal{H}_\phi$. In particular, because of Eq. (3.14), it satisfies: $\phi = d_{\tau_\phi}\phi * \phi$.

Obviously, $\mathcal{P}_1(G)$ contains more functions than just characteristic functions of the type (3.7). To identify which $\phi \in \mathcal{P}_1(G)$ are characteristic functions of states, first note that from Eq. (3.7) it follows that:

$$\phi_\varrho(g) = \sum_i p_i \langle \psi_i | \tau(g) \psi_i \rangle, \tag{3.16}$$

where we used any convex decomposition (for example an eigenensemble) of ϱ: $\varrho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. From Eq. (3.16), we see that the decomposition of ϕ_ϱ into extreme points from $\mathcal{E}_1(G)$ contains only one, fixed representation τ. Conversely, let $\phi = \sum_i p_i \phi_i$ where $\mathcal{E}_1(G) \ni \phi_i = \langle \psi_i | \tau \psi_i \rangle$ for each i (such sums are finite, since all irreducible representations are finite-dimensional), then $\phi = \phi_\varrho$, where $\varrho := \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

Let us describe the inverse non-commutative Fourier transform (3.10) of the whole $\mathcal{P}_1(G)$. Since G is compact, the set of its irreducible representations is discrete, and we can label them by some natural index k. Then, any $\phi \in \mathcal{P}_1(G)$ defines, through Eq. (3.10), a positive semidefinite operator $\varrho_k(\phi)$ for every irreducible

representation τ_k. To prove it, note that for any $|\psi\rangle \in \mathcal{H}_k$ (the space of τ_k) holds:

$$\begin{aligned}\langle\psi|\varrho_k(\phi)\psi\rangle &= \int \mathrm{d}g\ d_k\, \phi(g)\langle\psi|\tau_k(g)^\dagger\psi\rangle \\ &= \iint \mathrm{d}h\ \mathrm{d}g\ d_k\, \phi(h^{-1}g)\langle\tau_k(h)^\dagger\psi|\tau_k(g)^\dagger\psi\rangle \\ &= \sum_{\mu=1}^{d_k} \iint \mathrm{d}h\ \mathrm{d}g\ d_k\, \overline{\langle e_\mu|\tau_k(h)^\dagger\psi\rangle}\, \phi(h^{-1}g)\, \langle e_\mu|\tau_k(g)^\dagger\psi\rangle \geq 0. \end{aligned} \tag{3.17}$$

In the second step above we changed the variables $g \to h^{-1}g$, used the invariance of $\mathrm{d}g$, and inserted $1 = \int_G \mathrm{d}h$, since the integrand did not depend on h. Then we inserted a unit matrix, decomposed with respect to an arbitrary basis $\{|e_\mu\rangle\}$ of $\mathcal{H}_k$. However, generically $\varrho_k(\phi)$ is subnormalized as for a generic ϕ there appear all irreducible representations of G in the convex decomposition of ϕ into $\mathcal{E}_1(G)$. Hence, each $\phi \in \mathcal{P}_1(G)$ defines a positive semidefinite operator in the space $\bigoplus_k \mathcal{H}_k$, where the sum is over all irreducible representations of G, through:

$$\varrho(\phi) := \bigoplus_k \varrho_k(\phi), \tag{3.18}$$

while each $\varrho_k(\phi)$ is given by Eq. (3.10). Only such defined operator $\varrho(\phi)$ is normalized, which follows from the identity $\phi(g) = \sum_k \mathrm{tr}\big[\varrho_k(\phi)\tau_k(g)\big]$ (Folland [24]). Of course, if τ_k is not present in the decomposition of ϕ then, from Peter-Weyl Theorem 3.5, $\varrho_k(\phi) = 0$.

Summarizing, states on an irreducible representation space $\mathcal{H}_\tau$ are in the one-to-one correspondence with functions on G satisfying the conditions (3.8), (3.9), and (3.16). The last condition ensures that in the decomposition (3.18) there appears only the representation τ, and hence the operator given by Eq. (3.10) acts in the desired space and is normalized. The correspondence $\varrho \leftrightarrow \phi_\varrho$ may be heuristically viewed as a change of basis: $|e_\mu\rangle\langle e_\nu| \leftrightarrow \langle e_\nu|\tau(\cdot)e_\mu\rangle$. Note that one can also recover density matrices from their non-commutative characteristic functions using directly the GNS construction. If $\phi = \phi_\varrho$, so that ϕ is of the form (3.16), the vector $|\psi_\phi\rangle$ is the, so called, purification of ϱ. Although deeper and more general, the GNS construction is less explicit than the inverse non-commutative Fourier transform (3.10).

The potential significance of non-commutative characteristic functions for quantum systems, both mechanical and with finite dimensional Hilbert spaces, has been first, up to our knowledge, pointed out by Gu in Ref. [32]. However, no investigation of the separability problem was carried out there, as the work of Gu predates the paper of Werner [102]. On the other hand, standard characteristic functions played a crucial role in solving the separability problem for Gaussian states by Giedke *et al.* [28].

Finally, let us mention about one alternative approach. One can define an analog of coherent states for spin-j systems — the, so called, *spin coherent states* (Perelomov [72]):

$$|\theta,\varphi\rangle := \exp\left[\mathrm{i}\theta(\sin\varphi\, J^1 - \cos\varphi\, J^2)\right]|j,-j\rangle, \quad 0 \leq \theta < \pi,\ 0 \leq \varphi < 2\pi, \tag{3.19}$$

where $\mathbf{J} := (J^1, J^2, J^3)$ is the spin operator. One can then introduce the corresponding P-representation, analogously to Eq. (2.1):

$$\varrho = \int_{\mathbb{S}^2} \mathrm{d}\Omega \, P_\varrho(\theta, \varphi) \, |\theta, \varphi\rangle\langle\theta, \varphi|, \tag{3.20}$$

where $\mathrm{d}\Omega := \sin\theta \, \mathrm{d}\theta \mathrm{d}\varphi$ is the volume element on a sphere. The proof of existence of the representation (3.20) is very similar to the one from Section 2.2, but less technical, since now P_ϱ's are functions, not distributions. However, unlike the usual P-representation (2.1) and the non-commutative characteristic function (3.7), the spin-coherent P-representation is not uniquely determined by a state: in the decomposition of $P_\varrho(\theta, \varphi)$ over the spherical harmonics Y_{lm}, ϱ determines only terms with $l \leq 2j$. That is the reason why we introduced the non-commutative characteristic functions. Nevertheless, using the representation (3.20) Braunstein *et al.* estimated in Ref. [10] the size of a ball of separable states around the normalized identity, thus proving that the separable states are bulky in the set of all states. Another application of the spin-coherent P-representation we will show in Section 5.4.

3.3 Application to the study of entanglement

Having established the formalism, we proceed to reformulate the separability problem in terms of non-commutative characteristic functions. Let us consider a bipartite, finite dimensional system, described by a Hilbert space $\mathcal{H} := \mathbb{C}^m \otimes \mathbb{C}^n$. At this point, we arbitrarily identify the spaces $\mathbb{C}^m$ and $\mathbb{C}^n$ with two independent representation spaces $\mathcal{H}_\pi$, $\mathcal{H}_\tau$ of irreducible representations π, τ of some compact kinematical group G:

$$\mathbb{C}^m \equiv \mathcal{H}_\pi, \quad \mathbb{C}^n \equiv \mathcal{H}_\tau. \tag{3.21}$$

Of course, the group and the representations should be chosen to match the desired dimensions m, n. This is the only constraint we impose on G at this stage.

The identification (3.21), although mathematically always possible and non-unique, may seem arbitrary from the physical point of view. For instance, for a given system we could have chosen another kinematical group G', possessing suitable representations. This freedom may in fact turn out to be a big advantage of the formalism, as the choice of G can be optimized in each practical case. There is also a "universal" kinematical group $G = SU(2)$ — since it possesses irreducible representations in all possible finite dimensions, it can serve as a kinematical group for all finite dimensional systems. The results of the previous Section imply then that we can describe through the formulas (3.7) and (3.10) *all* states in *all* finite dimensions in terms of non-commutative characteristic functions on $SU(2)$. Thus, without a loss of generality, we may always treat our system as a system of (possibly artificial) independent spins $j_1 := (m-1)/2$ and $j_2 := (n-1)/2$.

Having done the identification (3.21), we can view the Hilbert space of the full system $\mathcal{H} = \mathcal{H}_\pi \otimes \mathcal{H}_\tau$ as a representation space of the product group $G \times G$ under the unitary representation T, defined as:

$$T(g_1, g_2) := \pi(g_1) \otimes \tau(g_2). \tag{3.22}$$

Representation T is irreducible as a representation of $G \times G$ [4] and moreover, every irreducible representation of $G \times G$ is of that form, up to unitary equivalence (see Folland [24] for the proof). Hence, we may view $G \times G$ as a kinematical group of the composite system. Since $G \times G$ is obviously compact, we can apply to it all the methods of the previous Section.

Let us consider a separable state ϱ on $\mathcal{H}_\pi \otimes \mathcal{H}_\tau$, for which there exists a convex decomposition of the type (3.3): $\varrho = \sum_i p_i |u_i\rangle\langle u_i| \otimes |v_i\rangle\langle v_i|$. Then, from Eq. (3.7) we obtain that:

$$\phi_\varrho(g_1, g_2) = \sum_i p_i \kappa_i(g_1)\eta_i(g_2), \tag{3.23}$$

where $\kappa_i(g_1) := \langle u_i|\pi(g_1)u_i\rangle$, $\eta_i(g_2) := \langle v_i|\tau(g_2)v_i\rangle$ are non-commutative characteristic functions from $\mathcal{P}_1(G)$, or more precisely from $\mathcal{E}_1(G)$. Conversely, a function of the form (3.23) defines a separable state through the integral (3.10), because:

$$\begin{aligned}&\int_{G\times G} \mathrm{d}g_1\mathrm{d}g_2 \; d_T\, \phi(g_1, g_2)T(g_1, g_2)^\dagger = \\ &= \sum_i p_i \left(\int_G \mathrm{d}g_1 \, d_\pi \kappa_i(g_1)\pi(g_1)^\dagger \right) \otimes \left(\int_G \mathrm{d}g_2 \, d_\tau \eta_i(g_2)\tau(g_2)^\dagger \right),\end{aligned} \tag{3.24}$$

where $\mathrm{d}g := \mathrm{d}g_1\mathrm{d}g_2$ is the Haar measure on $G \times G$. Moreover, since we need to integrate in Eq. (3.24) in order to obtain a density matrix, it is enough that the decomposition (3.23) holds almost everywhere with respect to the measure $\mathrm{d}g$. Hence we obtain the following theorem:

Theorem 3.7. *Let G be a compact kinematical group; π, τ its irreducible representations. A state ϱ on $\mathcal{H}_\pi \otimes \mathcal{H}_\tau$ is separable if and only if its non-commutative characteristic function ϕ_ϱ can be written as a convex combination: $\phi_\varrho(g_1, g_2) = \sum_i p_i \kappa_i(g_1)\eta_i(g_2)$, where $\kappa_i, \eta_i \in \mathcal{E}_1(G)$ and the equality holds almost everywhere with respect to the Haar measure on $G \times G$.*

The above Theorem is our group-theoretical reformulation of the separability problem. The generalization to arbitrary multipartite systems is straightforward. We call the functions possessing decompositions of the type (3.23) *separable* and otherwise — *entangled*. One may thus generalize the separability problem to groups in the following way:

Definition 3.4 (Generalized separability problem). *Given an arbitrary function $\phi \in \mathcal{P}_1(G \times G)$, decide whether it is separable or not.*

This is an interesting mathematical problem, with connections to e.g. properties of polynomials on groups: if $G = SU(2)$, then, since ϕ_ϱ are polynomials in the group parameters, Theorem 3.7 states that a state is separable iff its group polynomial separates into two polynomials in the variables g_1 and g_2 respectively.

[4] Obviously T becomes reducible when restricted to the diagonal subgroup $\{(g, g); g \in G\}$, but this does not concern us here.

One of the potential advantages of the current approach is its universality. For example, for $G = SU(2)$ a characterization of separable functions within $\mathcal{P}_1(SU(2) \times SU(2))$ would lead through Eqs. (3.10) and (3.18) to a characterization of separable states in all possible finite dimensions. The other conceptual advantage will be discussed in Section 3.7.

Note that if one considers a restriction $\phi|_{Abel}$ of an arbitrary $\phi \in \mathcal{P}_1(G \times G)$ to any Abelian subgroup of $G \times G$ (like the Cartan subgroup if G is a Lie group, i.e. its maximal torus), then the separable decomposition (3.23), possibly infinite, always exists. This follows from the fact that on Abelian groups the usual Fourier transform is available. That is, on Abelian groups Fourier transform assigns functions to functions. For a concrete example consider $G = SU(2)$. Then the maximal torus is $U(1) \times U(1)$ and one can always write:

$$\phi(\theta_1, \theta_2) = \sum_{k,l} (\mathcal{F}\phi)_{kl} \, \mathrm{e}^{-\mathrm{i}k\theta_1} \, \mathrm{e}^{-\mathrm{i}l\theta_2}, \tag{3.25}$$

where the angles θ_1, θ_2 parametrize $U(1) \times U(1)$ and $(\mathcal{F}\phi)_{kl}$ are the Fourier coefficients of $\phi|_{U(1)\times U(1)}$. Since $\mathrm{e}^{-\mathrm{i}k\theta} \in \mathcal{P}_1(U(1))$, $(\mathcal{F}\phi)_{kl} \geq 0$ by Bochner's Theorem 2.2, and $\sum_{kl}(\mathcal{F}\phi)_{kl} = 1$ by the normalization of ϕ (3.9), the Fourier series (3.25) is just a separable decomposition of $\phi|_{U(1)\times U(1)}$. For characteristic functions of states, i.e. for $\phi = \phi_\varrho$, the series (3.25) is finite: $k = -2j_1, -2j_1 + 2, \ldots, 2j_1$, $l = -2j_2, -2j_2 + 2, \ldots, 2j_2$, where j_1, j_2 are the corresponding spins, as ϕ_ϱ's are polynomials of bi-degree $(2j_1, 2j_2)$ in the group parameters; see Appendix A. However, for separable states the decomposition (3.25) will not generically prolong to the whole $SU(2) \times SU(2)$, as it contains at most $(2j_1+1)(2j_2+1) = mn$ terms, whereas from Caratheodory's Theorem (Theorem 3.3, Section 3.1), we know that the number of terms in a separable decomposition is bounded by m^2n^2. We further develop the connection between group non-commutativity and entanglement in Section 3.7.

3.4 Analysis of the PPT criterion and pure states

In this Section we analyze the group-theoretical version of the PPT criterion (Theorem 3.4) and the criterion given by Proposition 3.1, both introduced in Section 3.1.2. Recall that the PPT condition states that if ϱ is separable, then the partially transposed matrix ϱ^{T_1} is positive semidefinite[5].

Let us first note that for an arbitrary positive definite function ϕ it holds:

$$\phi(g^{-1}) = \overline{\phi(g)}, \tag{3.26}$$

and $\overline{\phi}$ is again positive definite, which follows from the GNS representation (3.15). Hence, we immediately obtain from Eq. (3.23) a necessary separability criterion for an arbitrary $\phi \in \mathcal{P}_1(G \times G)$:

[5]For definiteness' sake, we will transpose only with respect to the first party but our arguments, after obvious changes, hold equally well for transposition with respect to the second party too.

Proposition 3.2. *If* $\phi \in \mathcal{P}_1(G\times G)$ *is separable then* $\widetilde{\phi}(g_1,g_2) := \phi(g_1^{-1},g_2) \in \mathcal{P}_1(G\times G)$.

In particular, using Theorem 3.7 we obtain the implication: (ϱ - separable) $\Rightarrow \widetilde{\phi}_\varrho \in \mathcal{P}_1(G\times G)$. We will show that it is closely related to the PPT condition. For that we will first consider $G = SU(2)$:

Proposition 3.3. $\widetilde{\phi}_\varrho \in \mathcal{P}_1(SU(2)\times SU(2))$ *if and only if* $\varrho^{T_1} \geq 0$.

Proof. Let us first assume that $\varrho^{T_1} \geq 0$, so that $\phi_{\varrho^{T_1}} \in \mathcal{P}_1(SU(2)\times SU(2))$. The latter is just $\phi_{\varrho^{T_1}}(g_1,g_2) = \mathrm{tr}\big[\varrho\ \overline{\pi(g_1^{-1})}\otimes\tau(g_2)\big]$, and since for any $a\in SU(2)$

$$\bar{a} = uau^{-1}, \quad u := -i\sigma^y\,, \tag{3.27}$$

and π polynomially depends on the group parameters (see Appendix A), we obtain that $\phi_{\varrho^{T_1}}(g_1,g_2) = \phi_\varrho(ug_1^{-1}u^{-1},g_2)$. The positive definiteness condition (3.8) for $\phi_{\varrho^{T_1}}$ takes then the following form:

$$\begin{aligned}\iint \mathrm{d}\tilde{g}\,\mathrm{d}\tilde{h}\,\overline{f(\tilde{g})}\,\phi_{\varrho^{T_1}}(\tilde{g}^{-1}\tilde{h})f(\tilde{h}) = \int \mathrm{d}g_1\,\mathrm{d}g_2 \int \mathrm{d}h_1\,\mathrm{d}h_2 \\ \times\overline{f(g_1u,g_2)}\,\widetilde{\phi}_\varrho(g_1^{-1}h_1,g_2^{-1}h_2)\,f(h_1u,h_2)\geq 0,\end{aligned} \tag{3.28}$$

where $\tilde{g} := (g_1,g_2)$. Since the inequality (3.28) is satisfied for any $f\in L^1(SU(2)\times SU(2))$, the right shift by u of the first argument is irrelevant. Thus, we get that $\widetilde{\phi}_\varrho \in \mathcal{P}_1(SU(2)\times SU(2))$ (the normalization follows trivially).

On the other hand, let us assume that $\widetilde{\phi}_\varrho \in \mathcal{P}_1(SU(2)\times SU(2))$. Then from the similar argument to that leading to the property (3.17), we can construct a positive semidefinite operator:

$$\begin{aligned}&\int_{G\times G} \mathrm{d}g_1\mathrm{d}g_2\ d_T\,\widetilde{\phi}_\varrho(g_1,g_2)T(g_1,g_2)^\dagger = \\ &= \int \mathrm{d}g_1\,\mathrm{d}g_2\ d_\pi d_\tau\,\phi_\varrho(g_1,g_2)\,\overline{\pi(u)}\big[\pi(g_1)^\dagger\big]^T\pi(u)^T\otimes\tau(g_2)^\dagger \\ &= \big[\overline{\pi(u)}\otimes\mathbf{1}\big]\,\varrho^{T_1}\,\big[\pi(u)^T\otimes\mathbf{1}\big]\geq 0,\end{aligned} \tag{3.29}$$

where in the first step we used the fact that $\mathrm{d}g^{-1} = \mathrm{d}g$. Since the local unitary rotation by $\pi(u)^T\otimes\mathbf{1}$ does not affect the positivity of the operator in the inequality (3.29), the latter is equivalent to $\varrho^{T_1}\geq 0$. □

The crucial role in the above proof, especially in obtaining the inequality (3.29), has been played by the relation (3.27), implying the unitary equivalence, denoted by $\sim$, between $SU(2)$-representations τ_k and their complex conjugates $\overline{\tau_k}$ for all k: $\overline{\tau_k} = C_k\tau_kC_k^\dagger$, i.e. $\tau_k\sim\overline{\tau_k}$. Moreover, the intertwining isomorphisms C_k, equal to $\tau_k(u)$ for this particular group, satisfy $\overline{C_k}C_k = \mathbf{1}$. Representations with such properties are called representations of real type (Trautman [99]).

Now a natural question arises: if we consider a kinematical group which possesses at least one irreducible representation $\pi\not\sim\overline{\pi}$ (for example $G = SU(3)$, $\pi = \mathrm{id}$), can we obtain from Proposition 3.2 any new criterion, independent from the PPT condition? The negative answer provides the next Theorem:

Theorem 3.8. *Let G be a compact kinematical group; π, τ its irreducible representations. For any state ϱ on $\mathcal{H}_\pi \otimes \mathcal{H}_\tau$, $\varrho^{T_1} \geq 0$ if and only if $\widetilde{\phi}_\varrho \in \mathcal{P}_1(G \times G)$.*

Proof. For a general group G the property (3.27) does not hold and we cannot use the previous technique. However, $\widetilde{\phi}_\varrho$ can be represented as follows:

$$\widetilde{\phi}_\varrho(g_1, g_2) = \mathrm{tr}\big[\varrho^{T_1}\ \overline{\pi(g_1)} \otimes \tau(g_2)\big], \tag{3.30}$$

so that $\widetilde{\phi}_\varrho$ becomes a non-commutative characteristic function of ϱ^{T_1}, treated as an operator acting on $\mathcal{H}_{\overline{\pi}} \otimes \mathcal{H}_\tau$. Since $\overline{\pi}$ is irreducible if and only if π is, we can invert the transformation (3.30):

$$\varrho^{T_1} = \int_{G\times G} \mathrm{d}g_1 \mathrm{d}g_2\ d_\pi d_\tau\, \widetilde{\phi}_\varrho(g_1, g_2)\, \overline{\pi}(g_1)^\dagger \otimes \tau(g_2)^\dagger. \tag{3.31}$$

Then the statement follows immediately from the general results of Section 3.2: if $\widetilde{\phi}_\varrho \in \mathcal{P}_1(G \times G)$, positivity of ϱ^{T_1} follows from the same argument as that leading to the inequality (3.17). On the other hand, if $\varrho^{T_1} \geq 0$ then a direct calculation shows that $\widetilde{\phi}_\varrho$ satisfies the condition (3.8). □

Let us now briefly examine pure states. As we mentioned in Section 3.1, for pure states a number of necessary and sufficient separability conditions is available. The one which is most easily translated into the group-theoretical language is the one given by Proposition 3.1. Using the orthogonality of the matrix elements of irreducible representations (3.11), we easily obtain that that criterion is equivalent to the following integral condition:

Proposition 3.4. *A function $\phi \in \mathcal{E}_1(G \times G)$ is product if and only if:*

$$\int_G dg_1\ d_\pi\, |\phi(g_1, e)|^2 = 1 = \int_G dg_2\ d_\tau\, |\phi(e, g_2)|^2. \tag{3.32}$$

Note that the above condition applies to an *arbitrary* $\phi \in \mathcal{E}_1(G \times G)$ since, as we mentioned in Section 3.2, every $\phi \in \mathcal{E}_1(G \times G)$ is of the form ϕ_ψ f or some irreducible representation $\pi \otimes \tau$ of $G \times G$ and some pure state $|\psi\rangle \in \mathcal{H}_\pi \otimes \mathcal{H}_\tau$.

3.5 Analysis on finite groups

In this Section we study the special case of finite kinematical groups. An example of such groups are symmetric groups $\mathfrak{S}_M$ (groups of permutations of M elements). Moreover, every finite group is isomorphic to a subgroup of some $\mathfrak{S}_M$. Finite groups are in particular compact, and hence all the previous theory applies to them as well, with the only change being:

$$\int_G \mathrm{d}g \to \frac{1}{|G|} \sum_{g\in G}, \tag{3.33}$$

where $|G|$ is the number of elements of G (its order). However, for finite groups several simplifications occur. First of all, if $|G| = N$, then the space of complex

functions on G is isomorphic to $\mathbb{C}^N$, and we may identify each function ϕ with a row vector $\vec{\phi}$ of its values. The positive definiteness condition (3.8) takes then the following form:

$$\sum_{\alpha,\beta=1}^{N} \overline{c_\alpha}\phi(g_\alpha^{-1}g_\beta)c_\beta \geq 0 \quad \text{for any} \quad \vec{c}\in\mathbb{C}^N, \tag{3.34}$$

(indices $\alpha,\beta,\ldots$ now enumerate the group elements), which is just the positive semidefiniteness condition for the matrix:

$$\mathbf{\Phi}_{\alpha\beta} := \phi(g_\alpha^{-1}g_\beta) \tag{3.35}$$

(c.f. Theorem 2.2 from Section 2.3). To closer examine the structure of this matrix, let us first fix the labelling of the group elements such that $g_1 := e$. Then, the first row of $\mathbf{\Phi}$ contains the values of the function ϕ itself, and hence, it determines the rest of the matrix. We may define a function σ on $N\times N$ through:

$$g_{\sigma(\alpha,\beta)} := g_\alpha^{-1}g_\beta. \tag{3.36}$$

Note that σ is completely determined by the group multiplication table, $\sigma(\alpha,\alpha)=1$, and it satisfies the cocycle condition:

$$g_{\sigma(\alpha,\beta)}g_{\sigma(\beta,\gamma)} = g_{\sigma(\alpha,\gamma)} \tag{3.37}$$

(no summation over β here). Combining Eq. (3.36) with the normalization condition (3.9), and the property (3.26), we obtain the general form of the matrix (3.35) for an arbitrary $\phi\in\mathcal{P}_1(G)$:

$$\mathbf{\Phi} = \begin{bmatrix} 1 & \phi_2 & \phi_3 & \cdots & \phi_N \\ \overline{\phi_2} & 1 & \phi_{\sigma(2,3)} & \cdots & \phi_{\sigma(2,N)} \\ \overline{\phi_3} & \overline{\phi_{\sigma(2,3)}} & 1 & \cdots & \phi_{\sigma(3,N)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \overline{\phi_N} & \overline{\phi_{\sigma(2,N)}} & \overline{\phi_{\sigma(3,N)}} & \cdots & 1 \end{bmatrix}. \tag{3.38}$$

In other words, the matrix $\mathbf{\Phi}$ is built from the vector $\vec{\phi}$ by permuting in each row (or column) its components according to the multiplication table of G. Relabelling of the group elements corresponds to a unitary rotation of $\mathbf{\Phi}$, which does not affect the condition (3.34), and hence we may work with a fixed labelling.

For pure states, one can rewrite the convolution condition (3.14) in the following form:

$$\phi_\varrho(g^{-1}g') = \int_G \mathrm{d}h\, d_\tau\, \phi_\varrho(g^{-1}h)\phi_\varrho(h^{-1}g'), \tag{3.39}$$

from which it follows that ϱ is pure if and only if:

$$\mathbf{\Phi}_\varrho^2 = \frac{N}{d_\tau}\mathbf{\Phi}_\varrho. \tag{3.40}$$

Hence, the matrix $(d_\tau/N)\mathbf{\Phi}_\varrho$ is a projector.

Let us now move to bipartite systems, i.e. to systems with the kinematical group $G\times G$. We may view functions ϕ on such group either as $N\times N$ matrices $\phi_{\alpha\beta} := \phi(g_\alpha, g_\beta)$, or as vectors from $\mathbb{C}^{N^2}$. The separability criterion — Theorem 3.7 —, takes then the following form on finite G:

Proposition 3.5. *A function $\phi \in \mathcal{P}_1(G \times G)$ is separable if and only if there exists a convex decomposition:*

$$\phi_{\alpha\beta} = \sum_i p_i \, \kappa_{i\alpha} \, \eta_{i\beta}, \tag{3.41}$$

where for each i vectors $\vec{\kappa_i}$, $\vec{\eta_i} \in \mathbb{C}^N$ lead, according to the prescription (3.38), to positive semidefinite matrices.

Decomposition (3.41) resembles the singular value decomposition of the matrix $\phi_{\alpha\beta}$, however the vectors are specifically constrained. Let us mention another, equivalent form of Proposition 3.5:

Proposition 3.6. *A function $\phi \in \mathcal{P}_1(G \times G)$ is separable if and only if its matrix $\mathbf{\Phi}$, defined by Eq. (3.35), can be convexly decomposed as follows:*

$$\mathbf{\Phi} = \sum_i p_i \boldsymbol{K}_i \otimes \boldsymbol{N}_i, \tag{3.42}$$

where for each i, $\boldsymbol{K}_i, \boldsymbol{N}_i \geq 0$ and are of the form (3.38) for some $\vec{\kappa_i}, \vec{\eta_i} \in \mathbb{C}^N$.

The proof follows from the fact that the first row of the matrix equality (3.42) is just the Eq. (3.41), and from the specific structure (3.38) of the matrices in Eq. (3.42).

From the condition (3.34), the matrix $\mathbf{\Phi}_{\alpha\alpha',\beta\beta'} = \phi(g_\alpha^{-1} g_\beta, g_{\alpha'}^{-1} g_{\beta'})$ is positive semidefinite as an operator on $\mathbb{C}^N \otimes \mathbb{C}^N$, and, after rescaling by $1/N^2$, has trace one. Hence, Proposition 3.6 embeds the given separability problem into the higher dimensional one. For example, if one wants to study $3 \otimes 3$-dimensional separability problem, then the lowest order finite group, which possesses a three dimensional irreducible representation is the alternating group A_4 (the group of even permutations from $\mathfrak{S}_4$). Its order is $N = 12$ and Eq. (3.42) states then the separability problem in the dimension $12 \otimes 12$. Note however that the matrices in Eq. (3.42) are of a very specific form: they are completely determined by their first rows and the group multiplication table.

Finally, the group-theoretical version of the PPT criterion, given by Proposition 3.2, takes a particularly familiar from for finite groups:

Proposition 3.7. *If $\phi \in \mathcal{P}_1(G \times G)$ is separable then $\mathbf{\Phi}^{T_1} \geq 0$.*

The proof follows from Proposition 3.2, the equality:

$$\widetilde{\mathbf{\Phi}}_{\alpha\alpha',\beta\beta'} = \widetilde{\phi}(g_\alpha^{-1} g_\beta, g_{\alpha'}^{-1} g_{\beta'}) = \phi(g_\beta^{-1} g_\alpha, g_{\alpha'}^{-1} g_{\beta'}) = \mathbf{\Phi}_{\beta\alpha',\alpha\beta'},$$

and the positive definiteness condition (3.34).

3.6 Formal resemblance to local hidden variables models

Let us remark here on a purely formal resemblance of the group-theoretical formalism from the preceding Sections to LHV models, we mentioned in the Section 3.1. Following the usual approach (Bell [5], Werner and Wolf [104]), let us consider an expectation value of a product operator $A \otimes B$, where $A = \sum_\mu a_\mu P_\mu$, $B = \sum_\nu b_\nu Q_\nu$ are the corresponding spectral decompositions. Using the representation (3.10), the mean value of $A \otimes B$ in a state ϱ can be written as follows:

$$\mathrm{tr}(A \otimes B\varrho) = \sum_{\mu,\nu} a_\mu b_\nu \int_{G\times G} \mathrm{d}g_1\, \mathrm{d}g_2\; d_\pi d_\tau\, \phi_\varrho(g_1, g_2) \times \mathrm{tr}\big[P_\mu \pi(g_1)^\dagger\big]\, \mathrm{tr}\big[Q_\nu \tau(g_2)^\dagger\big]. \tag{3.43}$$

Hence, the probability $p_\varrho(\mu, \nu|A, B)$ of obtaining the value a_μ for A and b_ν for B, defined by the first equality in Eq. (3.2), is given by:

$$p_\varrho(\mu, \nu|A, B) = \int \mathrm{d}g_1 \mathrm{d}g_2\; d_\pi d_\tau\, \phi_\varrho(g_1, g_2) \mathrm{tr}\big[P_\mu \pi(g_1)^\dagger\big]\, \mathrm{tr}\big[Q_\nu \tau(g_2)^\dagger\big]. \tag{3.44}$$

This expression *formally* resembles an average in a LHV model, i.e. in a classical statistical model, where the role of the probability space plays $G \times G$, the "response functions" are $R(\mu, g_1) := \mathrm{tr}\big[P_\mu\, \pi(g)^\dagger\big]$ and $R(\nu, g_2) := \mathrm{tr}\big[Q_\nu\, \tau(g_2)^\dagger\big]$, and the "probability measure" is $\mathrm{d}m := d_\pi d_\tau\, \phi_\varrho(g_1, g_2)\, \mathrm{d}g_1 \mathrm{d}g_2$. The resemblance is of course only formal, since the "response functions", as well as the "probability measure" $\mathrm{d}m$, are complex (the response functions satisfy only $R(g^{-1}) = \overline{R(g)}$; see Section 4.4 of Chapter 4).

3.7 Non-commutativity and entanglement

We conclude with a general remark, connecting the very existence of entanglement with non-commutativity of the kinematical group G. For that we first have to change the usual mathematical language of quantum statistics (we do not consider dynamics here). Instead of using Hilbert spaces and density matrices, let us: i) assume that the kinematical arena is set up by the kinematical group G; ii) represent physical states by functions from $\mathcal{P}_1(G)$ (or its subset), rather than by density matrices; iii) for composite systems, take as the kinematical group the product group $G \times G \times G \ldots$ (for alternative group-theoretical reformulations of quantum mechanics see e.g. Mielnik [66], Gnutzmann and Kuś [30], Naudts and Kuna [69]). As we have seen in Section 3.2, such a description is indeed equivalent to the standard one, provided that the kinematical group is chosen correctly: for spin systems $G = SU(2)$, for canonically quantized particles it is the Heisenberg-Weyl group, as we will see in the next Chapter, while for classical particles G is just the phase-space $\mathbb{R}^{2n}$.

Now, let us assume that the kinematical group is Abelian. Then the following generalization of Bochner's Theorem 2.2 holds:

Theorem 3.9 (Bochner). *Let G be a locally compact Abelian group. Then normalized positive definite functions on G are in a one-to-one correspondence with probabilistic measures on the dual group $\hat{G}$.*

For a group G its dual $\hat{G}$ is defined as the space of all classes of irreducible representations of G. For Abelian groups, their duals also have a structure of an Abelian group; for example $\widehat{\mathbb{R}^{2n}} \simeq \mathbb{R}^{2n}$ (see Folland [24] for more details or Section 4.3.3). Thus, in the Abelian case, our states, i.e. functions from $\mathcal{P}_1(G)$, are in the one-to-one correspondence with probabilistic measures on $\hat{G}$. As a consequence, we recover the classical statistical description of our system, with $\hat{G}$ playing the role of the phase-space (at least for the purpose of statistics). If, moreover, the system under consideration is multipartite, then due to the fact that $\widehat{G_1 \times G_2} = \hat{G}_1 \times \hat{G}_2$ the phase-space of the composite system is the usual Cartesian product of the individual phase-spaces, and our states correspond to the probabilistic measures on this product. There is no place for entanglement here, understood as the impossibility of generating the composite system state-space from the individual state-spaces, because probabilistic measures on Cartesian products can always be decomposed (under suitable limits) into the convex mixtures of product measures (due to the underlying structure of the σ-algebra of Borel sets).

On the other hand, when G is non-Abelian, then Bochner's Theorem cannot be applied, and $\mathcal{P}_1(G)$ is in one-to-one correspondence with density matrices, or in other words with non-commutative probabilistic measures, through the inverse Frourier transform (3.10) and (3.18). Since density matrices exhibit entanglement, one may view the latter as the consequence of the non-commutativity of the kinematical group G. The last observation opens some possibility of speculations on the connection between entanglement and the uncertainty principles. In this context, we note that Gühne has developed in Ref. [33] some methods of entanglement description with the help of uncertainty relations.

3.8 The outlook

We will apply the general group-theoretical approach, sketched in the previous Section, to canonically quantized systems and the analysis of the correspondence principle in the next Chapter. It is also worth mentioning that this approach is somewhat related to the Loop Quantum Gravity programme (see e.g. Ashtekar and Lewandowski [3] and the references therein), where $SU(2)$ group and its irreducible representations play a fundamental role in describing quantum geometry of three-dimensional constant-time slices of space-time.

Another worth investigating direction is the analysis of bound entangled states using Propositions 3.5 and 3.6. Detection of bound entangled states has been rather a non-trivial task, due to their "proximity" to separable states. Because of the very special form of the matrices in Eq. (3.42), it might happen that the finite-group-theoretical version of the range criterion of Horodecki [40] would lead to some new, simpler tests.

Finally, as discussed at the end of Appendix A, the presented approach opens a possibility of deriving highly non-trivial statements on positive definite functions on products of non-Abelian groups, using the theory of entanglement. It might be thus of some use also for the mathematical field of harmonic analysis and non-commutative geometry.

Chapter 4

Group-theoretical formalism for quantum mechanical systems

In this Chapter we further generalize the method of characteristic functions from the previous Chapters. We sketch a group-theoretical framework, based on the Heisenberg-Weyl group, encompassing both quantum and classical statistical descriptions of mechanical systems. We redefine in group-theoretical terms the kinematical arena and the state-space of the system, achieving a unified statistical language and an elegant version of the quantum-classical correspondence principle. We briefly discuss the structure of observables and dynamics within the presented framework.

4.1 Introduction

Since the seminal works of Weyl [105] and Wigner [107], the fundamental role of group theory in quantum mechanics has become an established fact. The aim of the present Chapter is to point out that the group-theoretical reformulation of quantum statistics, proposed in Section 3.7, can be also applied to mechanical systems, and leads to: i) a unified language for quantum and classical statistical descriptions; ii) a natural limit $\hbar \to 0$, leading from a more generic quantum state-space to a classical one. The latter is an elegant and mathematically precise version of the quantum-to-classical correspondence principle at the level of statistical descriptions. Recall that by classical statistical description we understand the description based on probability measures on a phase-space, whereas by quantum - the one based on density matrices acting on a separable Hilbert space (Mackey [63]). Since the literature on the subject is enormous, let us state it clearly that this Chapter is neither meant to be an overview of the quantization methods, nor even an overview of the various forms of the correspondence principle. For that see e.g. Werner [103] or Landsman [58] and the references therein.

The change of mathematical representatives of kinematical arena and statistical states that we proposed in Section 3.7, was the following : as the kinematical arena

we consider a certain group G, which we called the *kinematical group*, together with its irreducible unitary representations[1]. As mathematical representatives of statistical states of the system we take the space $\mathcal{P}_1(G)$ of normalized positive definite functions on G — the non-commutative characteristic functions from Section 3.2. Obviously, the choice of the kinematical group G should be physically motivated if G is to play any fundamental role. In the previous Chapter we studied compact groups (e.g. $SU(2)$), which provide a natural framework for describing systems with finite dimensional Hilbert spaces (e.g. spin systems). In this Chapter, however, we would like to study mechanical systems (particles), so it is natural to expect that a good candidate for the kinematical group would be the Heisenberg-Weyl group (see e.g. Weyl [105], Folland [24], or Perelomov [72]) due to its fundamental role in kinematics of the standard quantum and classical mechanics. However, at the further stages of research more thorough operational argument should be given to motivate (or to abandon) this choice.

Hence, on one side, the formalism we develop in this Chapter is a generalization of the non-commutative characteristic functions from Chapter 3 to the non-compact group. On the other side, it is a generalization of the standard characteristic functions from Chapter 2 to the non-Abelian group. In fact, as we mentioned at the end of Section 3.2, this particular description of mechanical systems was initiated in physical literature by Gu in Ref. [32]. Especially in the context of providing a more coherent, as compared to the standard Wigner and Moyal functions, way of describing both quantum and classical statistics. However, Gu did not fully perform the reformulation of the theory and concentrated mostly on practical problems (like dynamics of multipartite mechanical systems), treating non-commutative characteristic functions rather as secondary objects with respect to the usual density matrices, just like we did in Chapter 3. Neither did he examine the representation of observables and the classical limit (on the level of kinematics) in the resulting formalism. Here, we explicitly carry over the mentioned conceptual change and treat from the beginning non-commutative characteristic functions as the primary objects of the theory, while density matrices or probability measures as the secondary. The resulting formalism is a modification of the standard Weyl quantization (Weyl [105]; see also e.g. Folland [23]). From another point of view, it is closely related to the approaches of Wigner [108] (see e.g. Schleich [87] for a modern exposition) and Moyal [68], for which $G = \mathbb{R}^{2n}$. It can also be treated as a special example of the abstract C^*-algebraic approach (see e.g. Haag [34] for a deep exposition and Landsman [58] for the latest trends). The classical limit, which appears in the presented formalism results from the structure of irreducible representations of the Heisenberg-Weyl group. This Chapter is based on our work [54].

[1]This should be contrasted with the "convex programme" of Mielnik [66], where a group also enters the formalism at a fundamental level. However, for Mielnik the relevant group is the group of dynamical motions.

4.2 The Heisenberg-Weyl group

The basic object of our study will be the Heisenberg-Weyl group, denoted by H_n. Here n is the number of degrees of freedom of the considered mechanical system. Thus, we fix the kinematical group: $G = H_n$. The group H_n can be identified with a space $\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$, equipped with the following multiplication law:

$$(s, \boldsymbol{\eta}, \boldsymbol{\xi}) \cdot (s', \boldsymbol{\eta}', \boldsymbol{\xi}') := \Big(s + s' + \frac{1}{2}\omega[(\boldsymbol{\eta}, \boldsymbol{\xi}), (\boldsymbol{\eta}', \boldsymbol{\xi}')], \boldsymbol{\eta} + \boldsymbol{\eta}', \boldsymbol{\xi} + \boldsymbol{\xi}' \Big), \tag{4.1}$$

where $(s, \boldsymbol{\eta}, \boldsymbol{\xi}) = (s, \eta_1, \ldots, \eta_n, \xi_1, \ldots, \xi_n)$ are the coordinates and:

$$\omega := \begin{pmatrix} 0 & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}. \tag{4.2}$$

In the sequel we will interchangeably denote group elements by $g, h, \ldots$ or by the corresponding coordinates. The Haar measure $\mathrm{d}g$ on H_n is just $\mathrm{d}s\, \mathrm{d}^n\boldsymbol{\xi}\, \mathrm{d}^n\boldsymbol{\eta}$. The irreducible, unitary, strongly continuous representations of H_n are characterized by the Stone-von Neumann Theorem (see e.g. Reed and Simon, vol. 1 [75] or Folland [24]). Let us briefly recall their structure, as they will play a crucial role in what follows. There is a family of infinite-dimensional representations T^λ , $\mathbb{R} \ni \lambda \neq 0$:

$$T^\lambda(s, \boldsymbol{\eta}, \boldsymbol{\xi}) := \mathrm{e}^{-\mathrm{i}\lambda s} \exp\Big[\frac{\mathrm{i}}{\lambda}(\eta_j \hat{q}_j - \xi_j \hat{p}_j)\Big] \tag{4.3}$$

(the repeated indices are summed over), where the self-adjoint generators $\hat{\mathbf{q}}, \hat{\mathbf{p}}$ satisfy on the common domain:

$$[\hat{q}_j, \hat{p}_k] = \mathrm{i}\lambda\delta_{jk}, \tag{4.4}$$

and a family of one-dimensional representations $T^0_{\mathbf{q},\mathbf{p}}$, labelled by $(\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2n}$:

$$T^0_{\mathbf{q},\mathbf{p}}(s, \boldsymbol{\eta}, \boldsymbol{\xi}) := \mathrm{e}^{\mathrm{i}(\eta_j q_j - \xi_j p_j)}. \tag{4.5}$$

From experiment we know that the physically relevant representation is $T^\hbar$ with $\lambda = \hbar$. Comparing the definitions (4.5) and (2.5), we see that $T^\hbar$ differs from the Weyl operators $W(\boldsymbol{\xi}, \boldsymbol{\eta})$ only by a phase factor $\mathrm{e}^{-\mathrm{i}\lambda s}$. As we will show, this seemingly small change makes quite a remarkable difference.

4.3 Group-theoretical reformulation

4.3.1 The approach of Wigner and Moyal

A search for a unified quantum and classical statistical description usually means a search for quantum analogs of classical probability distributions. In case of mechanical systems one traditionally follows Moyal [68], and defines a phase-space characteristic function (also known as the Moyal function) corresponding to a given density matrix ϱ by:

$$\chi_\varrho(\boldsymbol{\eta}, \boldsymbol{\xi}) := \mathrm{tr}\Big(\varrho \exp\Big[\frac{\mathrm{i}}{\hbar}(\eta_j \hat{q}_j - \xi_j \hat{p}_j)\Big]\Big) = \mathrm{tr}\big[\varrho\, W(\boldsymbol{\xi}, \boldsymbol{\eta})\big]. \tag{4.6}$$

Note the difference with respect to the definition of characteristic function (2.13) that we used in Chapter 2: Weyl operators in Eq. (4.6) are not normally ordered, and hence χ_ϱ differs from $\mathcal{F}P_\varrho$ by a factor $\exp\Big[(||\boldsymbol{\xi}||^2 + ||\boldsymbol{\eta}||^2)/2\Big]$. This definition turns out to be more convenient here. For example, since $\mathrm{tr}\varrho^2 < \infty$, χ_ϱ is square-integrable. The latter property guarantees that the Fourier transform of χ_ϱ — the Wigner function (Wigner [108], Moyal [68]):

$$W_\varrho(\mathbf{q},\mathbf{p}) := \int \frac{\mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}}{(2\pi\hbar)^{2n}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(\eta_j q_j - \xi_j p_j)}\chi_\varrho(\boldsymbol{\eta},\boldsymbol{\xi}), \tag{4.7}$$

is also a function from $L^2(\mathbb{R}^{2n})$, and not a (generically) highly singular object like $\mathcal{F}P_\varrho$. One then hopes that W_ϱ may serve as an analog of a classical phase-space probability distribution. However, this attempt fails, as it is a well known fact (see Wigner [108] or Schleich [87]) that the Wigner function (4.7) is generically not positive on $\mathbb{R}^{2n}$. On the other hand, there seems to be no universal relation between non-positivity of the Wigner function and a "genuine quantum behaviour" of density matrices: there are density matrices showing what is generally accepted as a "non-classical behaviour", and nevertheless possessing positive Wigner functions (for example, squeezed states, defined in Definitions 2.4 and 2.5 in Section 2.4).

There has been developed some methods to get around the above difficulty. One of them is to replace the abstract definitions (4.6) and (4.7) by operational ones, i.e. by ones involving prescribed interaction with an external reference particle. This allows one to construct a positive phase-space probability distribution (see e.g. Wódkiewicz [109]). Another way of producing a positive phase-space probability distribution is to use the coherent states $|\alpha\rangle$ and assign to each density matrix ϱ the Q-representation $\langle\alpha|\varrho\,\alpha\rangle$ (see e.g. Davidović and Lalović [14]).

4.3.2 The formalism of Weyl and its modification

In contrast to the approaches mentioned above, Weyl proposed to move in the opposite direction and assign with each Fourier-representable function:

$$F(\mathbf{q},\mathbf{p}) = \int \mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}\,\mathcal{F}F(\boldsymbol{\eta},\boldsymbol{\xi})\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\eta_j q_j - \xi_j p_j)} \tag{4.8}$$

an operator:

$$A_F^{Weyl} := \int \mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}\,\mathcal{F}F(\boldsymbol{\eta},\boldsymbol{\xi})\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\eta_j \hat{q}_j - \xi_j \hat{p}_j)} \tag{4.9}$$

Function F is then called the *symbol* of the operator A_F^{Weyl}. In order to recognize which functions lead through Eq. (4.9) to density matrices, observe that Moyal characteristic function (4.6) satisfies:

$$\iint \mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}\mathrm{d}^n\boldsymbol{\xi}'\mathrm{d}^n\boldsymbol{\eta}'\,\overline{f(\boldsymbol{\eta},\boldsymbol{\xi})}\mathrm{e}^{-\frac{\mathrm{i}}{2\hbar}\omega[(\boldsymbol{\eta},\boldsymbol{\xi}),(\boldsymbol{\eta}',\boldsymbol{\xi}')]}\chi_\varrho(\boldsymbol{\eta}'-\boldsymbol{\eta},\boldsymbol{\xi}'-\boldsymbol{\xi})f(\boldsymbol{\eta}',\boldsymbol{\xi}') \geq 0. \tag{4.10}$$

Hence it is not positive definite on $\mathbb{R}^{2n}$ (see Definition 2.3 of Section 2.3), which also explains the lack of positivity of the Wigner function.

The above feature of the Moyal characteristic function is, in our opinion, a drawback. To overcome it and to use more coherent notions in both quantum and classical regimes, Gu noted in Ref. [32] that if one replaces the standard definition (4.6) by a more logical one:

$$\phi_\varrho(g) := \mathrm{tr}\big[\varrho T^\hbar(g)\big] = \mathrm{e}^{-\mathrm{i}\hbar s}\chi_\varrho(\boldsymbol{\eta},\boldsymbol{\xi})\,, \tag{4.11}$$

then such defined function ϕ is positive-definite on H_n (see Definition 3.8, Section 3.2) and is also normalized. It is, of course, exactly the non-commutative characteristic function of ϱ, defined in the previous Chapter by Eq. (3.7), since ϱ acts on the representation space $\mathcal{H}_\hbar$ of H_n. The only difference is that now the kinematical group is non-compact.

Hence, following the approach outlined in Section 3.7, we propose the following alternative construction of quantum statistics of a mechanical system: i) treat the group H_n as the primitive entry of the formalism, which sets up the kinematical arena; ii) take as statistical states of the system, abstract at this moment, the space $\mathcal{P}_1(H_n)$ of normalized positive definite functions on H_n. The choice of the representations of states is motivated by the fact that both in classical and quantum cases characteristic functions possess the same features, provided they are properly defined through Eq. (4.11). In this Chapter by a "state" we will always mean a normalized positive definite function. However, the whole $\mathcal{P}_1(H_n)$ turns out to be too large.

To identify the set of physically relevant states within $\mathcal{P}_1(H_n)$ and recover the standard density matrix formalism, we use the GNS construction (Theorem 3.6, Section 3.2). Although this is the fundamental tool in algebraic approaches to quantum theory, note that here we are using it in a different manner. In particular, we are not starting from a C^*-algebra of observables, but rather from the kinematical group.

Recall that using the GNS construction we can uniquely (up to a unitary transformation) assign to each abstract state $\phi \in \mathcal{P}_1(H_n)$ a triple $(\mathcal{H}_\phi, \pi_\phi, |\psi_\phi\rangle)$, where π_ϕ is a representation of H_n acting in a Hilbert space $\mathcal{H}_\phi$, $|\psi_\phi\rangle$ is a normalized cyclic vector, and:

$$\phi(g) = \langle\psi_\phi|\pi_\phi(g)\,\psi_\phi\rangle\,. \tag{4.12}$$

The representation π_ϕ is generically reducible. As we mentioned in Section 3.2, it is irreducible if and only if ϕ is an extreme point of the state-space $\mathcal{P}_1(H_n)$, i.e. if and only if $\phi \in \mathcal{E}_1(H_n)$. Such states will be called *pure*. Motivated by the commutation relations (4.4), we call physical states those abstract states, for which π_ϕ is a countable multiple of $T^\hbar$: $\pi_\phi = \bigoplus_i T^\hbar$, $\mathcal{H}_\phi = \bigoplus_i \mathcal{H}_\hbar$, since then:

$$\phi(g) = \langle\psi_\phi|\bigoplus_i T^\hbar(g)\psi_\phi\rangle = \sum_i \langle\psi_i|T^\hbar(g)\psi_i\rangle = \mathrm{tr}[\widetilde{\varrho}_\phi T^\hbar(g)], \tag{4.13}$$

where $|\psi_i\rangle$'s are the components of $|\psi_\phi\rangle$ in each copy of $\mathcal{H}_\hbar$, and:

$$\widetilde{\varrho}_\phi := \sum_i p_i \big|\frac{\psi_i}{||\psi_i||}\big\rangle\big\langle\frac{\psi_i}{||\psi_i||}\big|\,, \quad p_i := ||\psi_i||^2\,, \quad \sum_i p_i = ||\psi_\phi||^2 = 1\,. \tag{4.14}$$

Hence, to each physical state ϕ we may assign a positive trace-class operator $\widetilde{\varrho}_\phi$ in $\mathcal{H}_\hbar$, representing ϕ. From Eqs. (4.3) and (4.13) we infer that physical states are of a special form:

$$\phi(s, \boldsymbol{\eta}, \boldsymbol{\xi}) = \mathrm{e}^{-\mathrm{i}\hbar s}\chi(\boldsymbol{\eta}, \boldsymbol{\xi}), \tag{4.15}$$

where χ is simply the standard Moyal characteristic function (4.6) of $\widetilde{\varrho}_\phi$.

The converse also holds, i.e. each abstract state ϕ of the form (4.15) is physical and we can uniquely assign to it a density matrix ϱ_ϕ (Gu [32]). Indeed, we can use the same integral (3.10) from Section 3.1 and define (c.f. Eq. (4.9)):

$$\varrho_\phi := \int_0^{\frac{2\pi}{\hbar}} \frac{\mathrm{d}s}{(2\pi)^2} \int \frac{\mathrm{d}^n\boldsymbol{\xi}\,\mathrm{d}^n\boldsymbol{\eta}}{(2\pi\hbar)^{n-1}}\, \phi(g)\, T^\hbar(g)^\dagger. \tag{4.16}$$

Since $\mathrm{tr}\Big(\exp\Big[\frac{\mathrm{i}}{\hbar}(\eta_j\hat{q}_j - \xi_j\hat{p}_j)\Big]\Big) = (2\pi\hbar)^n\,\delta^n(\boldsymbol{\xi})\delta^n(\boldsymbol{\eta})$, we have that:

$$\phi_{\varrho_\phi}(g) = \mathrm{tr}\big[\varrho_\phi T^\hbar(g)\big] = \phi(g), \tag{4.17}$$

and hence Eq. (4.16) can be viewed as the inverse non-commutative Fourier transform on H_n. Note that now we recover a function from an operator, and not vice versa like in Chapter 3. From Eq. (4.17) and the uniqueness of the GNS construction, it then follows that ϱ_ϕ is the same (up to unitary rotation) as the density matrix $\widetilde{\varrho}_\phi$ from Eq. (4.13). The representation (4.12) is recovered by spectrally decomposing ϱ_ϕ and then going back from Eq. (4.13) to Eq. (4.12). Moreover, if we look from the standard formalism point of view (c.f. Section 3.2), then we also have $\varrho_{\phi_\varrho} = \varrho$, (since matrix elements of T^λ satisfy orthonormality relations like matrix elements of an irreducible representation of a compact group; see Gu [32]).

Hence, physically relevant states are faithfully represented by $\phi \in \mathcal{P}_1(H_n)$ of the form (4.15)[2]. This specific form fixes the representations appearing in the GNS construction to the only physically relevant one with $\lambda = \hbar$. From now on we assume that we work only with physical states.

4.3.3 The classical limit

All that we have done above was just a reformulation of the standard theory. Density matrices are now secondary objects, constructed from the physical states and the proper representation of the kinematical group through Eq. (4.16) (or the GNS construction). We stress that we are dealing here with quantum *statistics* only, as the notion of the linear superposition seems not to be easily visible in the group-theoretical language. The main benefit of the presented reformulation lies, in our eyes, in that it provides a natural limit $\hbar \to 0$, in which one recovers classical statistics. Indeed, if we accept that what is experimentally available are density matrices (for example through the state tomography technique; see Section 5.6.1

[2]In fact, for establishing this correspondence we could have used only the formulas (3.8) and (4.16), but the GNS construction is more general - it can be carried out on an arbitrary locally compact group.

and Fig. 5.4), then we have to use the irreducible representations of the kinematical group in the limit $\hbar \to 0$ in order to recover them. As can be seen from Eq. (4.5), the irreducible representations of H_n become in this limit effectively the irreducible representations of the Abelian factorgroup $H_n/\{(s,0,0); s \in \mathbb{R}\} = \mathbb{R}^{2n}$, parametrized by $(\boldsymbol{\eta}, \boldsymbol{\xi})$. Hence, the states that we are naturally led to consider are now functions from $\mathcal{P}_1(\mathbb{R}^{2n})$. We do not have to worry about fixing the right, physical representation, like in Eq. (4.15), as it is already fixed by setting $\hbar = 0$ — these are the representations (4.5). The crucial point is that Bochner's Theorem (Theorem 3.9, Section 3.7) states that the functions from $\mathcal{P}_1(\mathbb{R}^{2n})$ are in the one-to-one correspondence with (Borel) probabilistic measures on the dual group $\widehat{\mathbb{R}^{2n}}$, isomorphic to $\mathbb{R}^{2n}$. The duality $\langle \cdot, \cdot \rangle$ is provided by the representation $T^0_{\mathbf{q},\mathbf{p}}$ itself: $\langle (\mathbf{q},\mathbf{p}), (\boldsymbol{\eta},\boldsymbol{\xi}) \rangle := T^0_{\mathbf{q},\mathbf{p}}(\boldsymbol{\eta},\boldsymbol{\xi})$ and $\widehat{\mathbb{R}^{2n}}$ is now parametrized by $(\mathbf{q},\mathbf{p})$. Thus, in the classical limit our states, i.e. functions $\phi \in \mathcal{P}_1(\mathbb{R}^{2n})$, can be uniquely identified with probabilistic measures μ_ϕ on $\widehat{\mathbb{R}^{2n}} \backsimeq \mathbb{R}^{2n}$ and the latter space plays the role of the classical phase-space of the system (at least in the context of statistical description). As a result, we recover classical statistical description of the system. It is also now clear why we did not identify the parameters of Weyl operators in Eq. (2.5) in Section 2.2 with the phase-space coordinates $(\mathbf{q},\mathbf{p})$: Weyl operators are parametrized by the dual object to the phase-space.

In the case that $\phi \in \mathcal{P}_1(\mathbb{R}^{2n})$ is also in $L^1(\mathbb{R}^{2n})$, or if we allow for distributions, we can explicitly recover μ_ϕ through the analog of the integral (4.16), which now becomes the usual Fourier transform (however we had to manually adjust the constant multiplying the measure):

$$\mathrm{d}\mu_\phi = (\mathcal{F}\phi)\, \mathrm{d}^n\mathbf{q}\mathrm{d}^n\mathbf{p}\,, \tag{4.18}$$

$$\begin{aligned} \mathcal{F}\phi(\mathbf{q},\mathbf{p}) &= \int \frac{\mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}}{(2\pi)^{2n}}\, \phi(\boldsymbol{\eta},\boldsymbol{\xi})\, T^0_{\mathbf{q},\mathbf{p}}(g)^\dagger \\ &= \int \frac{\mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}}{(2\pi)^{2n}}\, \phi(\boldsymbol{\eta},\boldsymbol{\xi})\, \mathrm{e}^{-\mathrm{i}(\eta_j q_j - \xi_j p_j)}, \end{aligned} \tag{4.19}$$

and $\mathcal{F}\phi$ is a classical probability density in the phase-space.

As a side remark, note that the presented approach can be also reformulated in the C^*-algebraic language: for a locally compact kinematical group G, the convolution algebra $L^1(G)$ can be equipped with a norm:

$$||f||^2_* := \sup_{\phi \in \mathcal{E}_1(G)} \iint \mathrm{d}g\, \mathrm{d}h \overline{f(g)} \phi(g^{-1}h) f(h) \tag{4.20}$$

turning it (after completion) into a C^*-algebra denoted by $C^*(G)$ (see e.g. Dixmier [17]). Then, each $\phi \in \mathcal{P}_1(G)$ defines a positive functional on $C^*(G)$ with a unit norm: $||\phi||_* = 1$. Thus, it defines a state in the algebraic terminology. In this reformulation, the role of the (usually abstract) C^*-algebra of observables is played by the group C^*-algebra $C^*(G)$. However, in the usual, abstract C^*-algebraic approach the notion of the classical limit is a priori not given and one has to build it into the theory "by hand" e.g. through the, so called, deformation quantization approach (see

e.g. Landsman's review [58] and the references therein). Actually, the presented approach can be also viewed as a concrete realization of the deformation quantization approach[3].

4.4 Remarks on observables and dynamics

In this Section we briefly describe the representation of observables and dynamics in our group-theoretical language. We will not be very detailed and mathematically strict here, but rather present a general outline. The easiest observables to deal with are those represented by trace-class operators in the standard language. In our reformulation they are given by complex continuous functions F from $L^1(S_n)$, where $S_n := [0, 2\pi/\hbar] \times \mathbb{R}^{2n} \subset H_n$, satisfying:

$$F(g^{-1}) = \overline{F(g)}. \tag{4.21}$$

The mean value of F in a state ϕ is defined as:

$$\langle F \rangle_\phi := \int_{S_n} \mathrm{d}g\, \phi(g) F(g)\,, \tag{4.22}$$

where we have rescaled dg so that it is now equal to $\mathrm{d}g = \left[(2\pi)^2(2\pi\hbar)^{n-1}\right]^{-1} \times \mathrm{d}s\, \mathrm{d}^n\boldsymbol{\xi}\, \mathrm{d}^n\boldsymbol{\eta}$. The integral (4.22) is well defined due to the boundedness of ϕ. To establish the connection with the standard representation of an observable, note that to each such F we can assign a hermitian operator A_F by a formula analogous to Eq. (4.16) (compare also with Eq. (4.9)):

$$A_F := \int_{S_n} \mathrm{d}g F(g) T^\hbar(g). \tag{4.23}$$

The above integral exists, in the sense of matrix elements, as $F \in L^1(S_n)$. On the other hand, to each trace-class observable A we can assign a continuous function F_A by an analog of Eq. (3.8):

$$F_A(g) := \mathrm{tr}[A T^\hbar(g)^\dagger]. \tag{4.24}$$

Using the same arguments as in the case of density matrices, one can easily show that $F_{A_F} = F$ and $A_{F_A} = A$, thus establishing the correspondence between trace-class observables and functions satisfying Eq. (4.21).

In the case of observables not representable by trace-class operators, one has to allow for distributions. We will not investigate here which exactly distribution space one needs to consider in order to cover all relevant observables, but only write down

[3] $C^*(G)$ is fibrated over $\mathbb{R}$, where the fibres are labelled by the representation parameter λ. For $\lambda = 0$, i.e. in the classical limit, the corresponding algebra is commutative, which follows from Eq. (4.5), and represents classical observables on $\mathbb{R}^{2n}$; see also the next Section.

the distributions $F_{\hat{q}_j}$ and $F_{\hat{p}_j}$ representing the generators $\hat{q}_j$ and $\hat{p}_j$:

$$\begin{aligned} F_{\hat{q}_j}(s,\boldsymbol{\eta},\boldsymbol{\xi}) &= \mathrm{i}\hbar\,(2\pi\hbar)^n \exp\Big[\mathrm{i}\hbar s - \frac{\eta_j^2}{4\hbar}\Big] \\ &\quad \times \delta^n(\boldsymbol{\xi})\delta(\eta_1)\ldots\frac{\partial}{\partial\eta_j}\delta(\eta_j)\ldots\delta(\eta_n) \qquad (4.25) \\ F_{\hat{p}_j}(s,\boldsymbol{\eta},\boldsymbol{\xi}) &= -\mathrm{i}\hbar\,(2\pi\hbar)^n \exp\Big[\mathrm{i}\hbar s - \frac{\xi_j^2}{4\hbar}\Big] \\ &\quad \times \delta^n(\boldsymbol{\eta})\delta(\xi_1)\ldots\frac{\partial}{\partial\xi_j}\delta(\xi_j)\ldots\delta(\xi_n). \qquad (4.26) \end{aligned}$$

Higher order polynomials in $\hat{q}_j$ and $\hat{p}_j$ are proportional to the higher order derivatives of Dirac's delta.

Let us now consider the representation of dynamics. The dynamical law takes a form of a differential equation imposed on a path $t \mapsto \phi_t$, which should be equivalent to the von Neumann equation for the corresponding density matrix ϱ_t:

$$\mathrm{i}\hbar\frac{\partial\varrho_t}{\partial t} = [H, \varrho_t]. \qquad (4.27)$$

In fact, such equation was derived and analyzed by Gu in Ref. [32] and we merely quote it here:

$$\mathrm{i}\hbar\frac{\partial\phi_t}{\partial t} = \left[H\Big(-\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{\eta}} + \frac{1}{2}\boldsymbol{\xi},\, \mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{\xi}} + \frac{1}{2}\boldsymbol{\eta}\Big) - H\Big(-\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{\eta}} - \frac{1}{2}\boldsymbol{\xi},\, \mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{\xi}} - \frac{1}{2}\boldsymbol{\eta}\Big)\right]\phi_t\,, \qquad (4.28)$$

where $H(\boldsymbol{q},\boldsymbol{p})$ is the Hamiltonian, which we assume to be of the form $T(\boldsymbol{p}) + V(\boldsymbol{q})$ to avoid the ordering problems. Note that due to the property (4.15), Eq. (4.28) is, modulo the phase factor, just the quantum Liouville equation (see e.g. Schleich [87]), but imposed on the characteristic function $\chi(\boldsymbol{\eta},\boldsymbol{\xi})$ rather than on the Wigner function $W(\mathbf{q},\mathbf{p})$:

$$\mathrm{i}\hbar\frac{\partial\chi_t}{\partial t} = \left[-\frac{\eta_j}{m}\frac{\partial}{\partial\xi_j} - \mathrm{i}\sum_{n=0}^{\infty}\frac{(\hbar/2)^{2n}}{(2n+1)!}\left(\frac{\xi_j}{\hbar}\frac{\partial}{\partial q_j}\right)^{2n+1} V\Big(\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{\eta}}\Big)\right]\chi_t\,, \qquad (4.29)$$

where we further assumed that $H(\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{p}^2/2m + V(\boldsymbol{q})$ and the potential $V(\boldsymbol{q})$ is an analytical function of $\boldsymbol{q}$.

In the classical limit, as we have argued before, the kinematical group effectively collapses to $\mathbb{R}^{2n}$ and observables become functions (or distributions) on $\mathbb{R}^{2n}$. The condition (4.21) now reads:

$$F(-\boldsymbol{\eta},-\boldsymbol{\xi}) = \overline{F(\boldsymbol{\eta},\boldsymbol{\xi})}, \qquad (4.30)$$

and from Eqs. (4.23) and (4.5) we obtain that:

$$A_F(\boldsymbol{q},\boldsymbol{p}) = \int\frac{\mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}}{(2\pi)^{2n}}\,F(\boldsymbol{\eta},\boldsymbol{\xi})\mathrm{e}^{-\mathrm{i}(\eta_j q_j - \xi_j p_j)}. \qquad (4.31)$$

Thus, observables correspond now to real (because of the condition (4.30)) functions on the phase-space $\widehat{\mathbb{R}^{2n}}$. Using Eqs. (4.18), (4.19), and (4.31) the state average (4.22) becomes simply the average of $A_F(\boldsymbol{q},\boldsymbol{p})$ with respect to the measure μ_ϕ, defined by the state in question ϕ:

$$\langle F\rangle_\phi = \int \frac{\mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}}{(2\pi)^{2n}}\, F(\boldsymbol{\eta},\boldsymbol{\xi})\,\phi(\boldsymbol{\eta},\boldsymbol{\xi}) = \int \mathrm{d}\mu_\phi(\boldsymbol{q},\boldsymbol{p}) A_F(\boldsymbol{q},\boldsymbol{p}). \tag{4.32}$$

To complete the picture, note that in the classical limit the dynamical law (4.29) reproduces, after rescaling: $\boldsymbol{\eta}\to\hbar\boldsymbol{\eta}$, $\boldsymbol{\xi}\to\hbar\boldsymbol{\xi}$ (see the next Section), the classical Liouville equation for a characteristic function:

$$\frac{\partial\phi_t}{\partial t} = -\left[\frac{\eta_j}{m}\frac{\partial}{\partial\xi_j} + \mathrm{i}\xi_j\frac{\partial V}{\partial q_j}\left(\mathrm{i}\frac{\partial}{\partial\boldsymbol{\eta}}\right)\right]\phi_t. \tag{4.33}$$

4.5 Examples of classical limits

Here we briefly show with two physical examples how the procedure of taking the limit $\hbar\to 0$ works in practice. However, let us stress again that it is not our goal to develop another tool for studying classical limits of quantum states, but rather to examine how the formalism of non-commutative characteristic functions leads to the more coherent quantum-classical language and the natural description of the correspondence principle. Since concrete examples of physically interesting states has been available to us in terms of density matrices ϱ anyway, we have to start from them. From this perspective, our approach obviously brings nothing new to the standard methods of Wigner and Moyal functions, as can it be seen from the form of physical states Eq. (4.15). Thus, we repeat that the main gain from the presented approach is conceptual rather than practical.

The prescription for taking classical limits is rather simple: use the basic formula (3.8) to calculate ϕ_ϱ for a given matrix ϱ. Next, check if there exists, in the distributive sense, a limit $\lim_{\hbar\to 0}\phi_\varrho$ (point limits are too restrictive). If a state ϕ is to possess a classical limit at all, we naturally expect that $\left(\lim_{\hbar\to 0}\phi\right)\in\mathcal{P}_1(\mathbb{R}^{2n})$, or in other words $\left(\lim_{\hbar\to 0}\phi\right)$ should be a classical characteristic function. If that is the case, we can use the prescription (4.18-4.19) to retrieve the corresponding probability measure. If not, i.e. $\lim_{\hbar\to 0}\phi$ does not exists, or is not in $\mathcal{P}_1(\mathbb{R}^{2n})$, then the state in question does not possess the classical limit.

To illustrate the procedure, let us first consider classical states, defined in Definition 2.1 in Section 2.1:

$$\varrho = \int_{\mathbb{R}^2}\mathrm{d}\mu(\alpha,\overline{\alpha})|\alpha\rangle\langle\alpha|, \tag{4.34}$$

where μ is a probabilistic measure on the classical phase-space $\mathbb{R}^2$. We stress that we consider coherent states here purely kinematicaly, without any explicit or implicit relation to the dynamics. They are defined as the states minimizing the Heisenberg uncertainty relations, arising from Eq. (4.4) and their particular importance for quadratic Hamiltonians does not concern us here.

Substituting Eq. (4.34) into Eq. (3.8) we obtain:

$$\phi_\varrho(s,\eta,\xi) = \int \mathrm{d}\mu(q,p)\,\mathrm{e}^{-\mathrm{i}\hbar s}\exp\left[-\frac{1}{4\hbar}(\xi^2+\eta^2)+\frac{\mathrm{i}}{\hbar}(q\eta-p\xi)\right]. \tag{4.35}$$

At a first glance, the last term in the integrand in Eq. (4.35) does not seem to possess any meaningful distributive limit when $\hbar \to 0$. That would be quite counterintuitive, as the matrices of the form (4.34) show a classical-like behaviour: for example the averages of normally ordered observables are equal to the phase-space averages with respect to μ. However, note that the parameters η, ξ are just some arbitrary coordinates on the Heisenberg-Weyl group and we are free to rescale them. Actually, the specific form of the operator $T^\hbar$ in Eq. (4.3) was motivated by the physical dimensional analysis (the argument of the exponential function should be physically dimensionless) and in order to recover the group multiplication law (4.1) one has to rescale $(\boldsymbol{\eta}, \boldsymbol{\xi})$ by $\hbar$. From another point of view, this rescaling is suggested by the Wigner function (4.7), which can be rewritten as follows:

$$W_\varrho(\mathbf{q},\mathbf{p}) = \int \frac{\mathrm{d}^n\boldsymbol{\xi}\mathrm{d}^n\boldsymbol{\eta}}{(2\pi)^{2n}}\mathrm{e}^{-\mathrm{i}(\eta_j q_j - \xi_j p_j)}\chi_\varrho(\hbar\boldsymbol{\eta},\hbar\boldsymbol{\xi}). \tag{4.36}$$

If we accept the above arguments, we are led to consider:

$$\lim_{\hbar\to 0}\phi(s,\hbar\eta,\hbar\xi) \tag{4.37}$$

instead of $\lim_{\hbar\to 0}\phi(s,\eta,\xi)$ as the proper classical limit (compare to the methods of Davidović and Lalović [14]). Then from Eq. (4.35) we obtain that:

$$\phi_\varrho(s,\hbar\eta,\hbar\xi) \xrightarrow[\hbar\to 0]{} \mathcal{F}\mu(\eta,\xi) = \int \mathrm{d}\mu(q,p)\,\mathrm{e}^{\mathrm{i}(q\eta-p\xi)}. \tag{4.38}$$

By Bochner's Theorem (or by an easy direct inspection) $\hat{\mu} \in \mathcal{P}_1(\mathbb{R}^2)$ and obviously the corresponding probability measure is just the measure μ itself, as one would expect.

As the next example let us consider the Fock states $|m\rangle$: $\varrho = |m\rangle\langle m|$. Again, we consider them just as kinematical examples. From Eq. (3.8) we obtain that:

$$\phi_\varrho(s,\eta,\xi) = \mathrm{e}^{-\mathrm{i}\hbar s}\mathrm{e}^{-\frac{1}{4\hbar}(\xi^2+\eta^2)}L_m\left[\frac{1}{2\hbar}(\xi^2+\eta^2)\right], \tag{4.39}$$

where $L_m(x) = m!\sum_{k=0}^m (-1)^k x^k/[(m-k)!(k!)^2]$ is the m-th order Laguerre polynomial. Just for illustration's sake, we will considered here a rather uninteresting limit $\hbar \to 0$ of a fixed Fock state $m = \text{const}$. Obviously, this limit does not have much physical sense, but from a *purely formal* point of view the vectors $|m\rangle$ are legitimate states in the kinematical space $L^2(\mathbb{R})$ and it is a legitimate question to ask what are their classical limits. Using the prescription (4.37) we obtain that:

$$\phi_\varrho(s,\hbar\eta,\hbar\xi) \xrightarrow[\hbar\to 0]{} 1, \tag{4.40}$$

which is trivially a function from $\mathcal{P}_1(\mathbb{R}^2)$. Hence, after performing the Fourier transform of (4.40), all the matrices $|m\rangle\langle m|$ are mapped in the classical limit to the same probability measure $\delta(q)\delta(p)$. Of course, one would expect that from the form of the energy spectrum of a harmonic oscillator, but as we said before, we consider the limit (4.40) only as a formal exercise. The physically sensible classical limit of the Fock states is given by $\hbar \to 0$, $m \to \infty$, $\hbar m = \text{const}$. In this limit one indeed recovers the classical microcanonical distribution function of the harmonic oscillator, as it was proven by Ripamonti in Ref. [79] using the closely related method of Wigner functions.

4.6 Concluding remarks

The next logical step would be to try to apply the developed formalism to systems with compact kinematical groups, like, for example, spin systems with $G = SU(2)$. The goal would be to describe the well known heuristic prescription: $\hbar \to 0$, $j \to \infty$, $j\hbar = \text{const}$, where j labels the irreducible representations of $SU(2)$, within the presented group-theoretical formalism.

Another point is that, at this stage, our approach lacks a clear operational meaning of the mathematical concepts involved. Perhaps the most operationally flavoured reformulation of quantum theory is the one given by the quantum logic and orthomodular lattices (see Mackey [63], or Beltrametti and Cassinelli [6] for an introduction), as it operates directly with the probabilities of outcomes of (idealized) measurements. It also very coherently incorporates classical and quantum statistics within a common language. However, it comes with its own set of problems: the justification for the use of Hilbert spaces for building the lattice and the apparent lack of a clear correspondence principle within the formalism. Note that another problem: the justification for the lattice orthomodularity, was solved only very recently by Grinbaum [31], using information-theoretical arguments of Rovelli [81].

Summarizing, the described approach presents an alternative to the standard as well as to the algebraic and lattice approaches to quantum statistics. It incorporates an elegant form of the correspondence principle. By the latter we mean a clear mechanism of showing how the classical state-space arises from the quantum one.

Chapter 5

Generalized spin squeezing inequalities in N qubit systems

In this Chapter we apply the method of entanglement witnesses to study quantum correlations in multiqubit systems, i.e. in complex systems built from elementary subsystems described by two dimensional Hilbert spaces. Our goal is to develop tests for multipartite entanglement using small number of experimentally available quantities. As such, we have chosen fluctuations of the total spin. We derive here inequalities that generalize the concept of the spin squeezing parameter and provide necessary and sufficient conditions for genuine 2-, or 3- qubit entanglement for symmetric states, and sufficient condition for general N-qubit states. We apply our method to a theoretical study of Dicke states. Then, we analyze the recently experimentally generated 7- and 8-ion W-states [Häffner *et al.* , Nature **438**, 643 (2005)]. Finally, we construct simplified criteria for detection of genuine tripartite entanglement.

5.1 Introduction

5.1.1 Some terminology

Apart from bipartite entanglement, introduced in Section 3.1, in this Chapter we will also study tripartite one. Since the latter is more complicated than the bipartite entanglement, let us briefly introduce the terminology.

Definition 5.1. *A state ϱ acting on $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ is called:*
• *fully separable if it can be represented as a convex combination of projectors onto product vectors of the type $|u\rangle_1 \otimes |v\rangle_2 \otimes |w\rangle_3$;*
• *biseparable if it can be represented as a convex combination of projectors onto vectors, which are product with respect to an arbitrary partition of the systems, i.e. vectors of the form $|\psi\rangle_{12} \otimes |u\rangle_3$, $|x\rangle_{13} \otimes |v\rangle_2$, and $|w\rangle_1 \otimes |y\rangle_{23}$;*
• *genuine tripartite entangled if neither of the above holds.*

By analogy, one can define various entanglement types for states of arbitrary many parties.

For systems of three qubits, i.e. when $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}_3 = \mathbb{C}^2$, genuine tripartite entangled states can be further classified with respect to their behaviour under local invertible transformations (Dür *et al.* [19], Acín *et al.* [2]). This classification is based on two important examples of genuine multipartite entangled pure states of N qubits: W-state:

$$|W_N\rangle := \frac{1}{\sqrt{N}}\Big(|100\cdots0\rangle + |010\cdots0\rangle + \cdots + |000\ldots1\rangle\Big), \tag{5.1}$$

and GHZ-state:

$$|GHZ_N\rangle := \frac{1}{\sqrt{2}}\Big(|000\cdots0\rangle + |111\cdots1\rangle\Big), \tag{5.2}$$

defined with respect to some basis $\{|0\rangle, |1\rangle\}$ of $\mathbb{C}^2$. Dür *et al.* showed in Ref. [19] that pure, genuine entangled states of 3-qubits fall into two inequivalent classes: W-type vectors, which can be locally converted into $|W_3\rangle$, and GHZ-type vectors, which can be locally converted into $|GHZ_3\rangle$. Hence, genuine tripartite entangled mixed states of 3-qubits also fall into two types: W-type entangled states, which are convex sums of projectors onto W-type vectors, and GHZ-type entangled states, which are convex sums of projectors onto GHZ-type vectors.

5.1.2 Motivation

Experimental generation and characterization of entanglement on a macroscopic, or mesoscopic scales seem to be one of the necessary prerequisites of scalable quantum information processing. A spectacular progress has been achieved recently in the area of quantum correlated systems of atoms, and in particular *macroscopic atomic ensembles*[1]. The main goal of these studies is to achieve an efficient quantum interface between light and atoms with spin, or pseudo-spin internal states, using the generalized quantum Faraday effect. Such settings already allowed one to demonstrate entanglement of distant atomic objects (Julsgaard *et al.* [44]), or deterministic memory for light (Julsgaard *et al.* [45]) that can be retrieved using quantum teleportation (Vaidman [100], Braunstein *et al.* [9]). Entanglement between light and atoms, and between atoms themselves plays, of course, essential role in these experiments.

It worth stressing that the light-atoms interface based on using the quantum Faraday effect does not only allow one to measure and detect atomic states. It does also provide a tool for manipulations and engineering of quantum fluctuations of atomic spins. The latter possibility might be of fundamental importance for the future implementations of distributed quantum information processing. In particular, the methods of atomic ensembles can be carried over to another rapidly developing

[1] For pioneering experimental work, see Hald *et al.* [35]; for very recent experiments on quantum feedback control, see Geremia *et al.* [27]; for the recent review of spin squeezing using Gaussian states, see Madsen and Mølmer [64].

area of ultracold atomic gases. Here, the interest would be to measure, characterize, and finally engineer quantum fluctuations of the total atomic spin in spinor ultracold gases (for a review see Stamper-Kurn and Ketterle [93]) that has been intensively studies since the seminal theory papers of Ho [37] and Ohmi and Machida [71], as well as the experiments performed by the MIT group on optically trapped sodium Bose-Einstein condensates (BEC) (Stenger *et al.* [94]).

Yet another rapidly developing related area is that of quantum information processing with trapped ions. After the first works, in which the 3- and 4-ion GHZ-state (Sackett *et al.* [85], Liebfried *et al.* [59]), and 3-ion W- and GHZ-state (Roos *et al.* [80]) have been generated, in recent experiments the tomography of 6-, 7-, and 8-ion W-states has been performed (Häffner *et al.* [36]), and the 6-ion GHZ-state has been generated (Liebfried *et al.* [60]).

5.1.3 Spin squeezing parameter

The problem of characterization of the generated forms of multipartite entanglement, or more generally, of characterization of many-body quantum correlations, is thus of essential importance for the investigations of such mesoscopic systems. One of the possible ways to achieve it, is to measure the total spin $\mathbf{J}$ (or pseudo-spin) of atoms (or ions) and its quantum fluctuations. The total spin is defined as follows:

$$J^i := \sum_{a=1}^{N} \frac{1}{2}\sigma_a^i \ , \quad i = 1, 2, 3 \tag{5.3}$$

(in this Chapter we work in the units $\hbar = 1$), where by σ^i we denote Pauli matrices, indices $a, b, c \ldots$ enumerate the particles of the ensemble, and $\sigma_a^i := \sigma^i \otimes \mathbf{1}_{1\ldots\hat{a}\ldots N}$ (hat over the index denotes that it is omitted). The central role in this approach, applied to atomic ensembles, has been played so far by the, so called, spin squeezing parameter ξ^2, defined by Kitagawa and Ueda in Ref. [46]. We introduce it through the following definition of squeezing for spin systems (c.f. Definitions 2.4 and 2.5, Section 2.4):

Definition 5.2. *A state of a spin-j system is called spin squeezed if there exists a direction* $\mathbf{n}$*, orthogonal to the mean spin* $\langle \mathbf{J} \rangle$*, such that:*

$$\xi^2 := 2\langle (\Delta J_{\mathbf{n}})^2 \rangle / j < 1, \tag{5.4}$$

where $J_{\mathbf{n}} := \mathbf{n} \cdot \mathbf{J}$*.*

The motivation for the above Definition, as well as for standard Definitions 2.4 and 2.5, is that squeezed states have smaller fluctuations of some particular observable (or along some particular direction) than the corresponding coherent states $|\theta, \varphi\rangle$ (see Eq. (3.19)) or $|\alpha\rangle$, which by definition optimize the relevant Heisenberg uncertainty relations. For spin systems, spin coherent states $|\theta, \varphi\rangle$ optimize the uncertainty relation: $\Delta J^1 \Delta J^2 \geq \hbar j/2$, originating from the commutation rule: $[J^1, J^2] = \mathrm{i} J^3$.

As it was shown by Sørensen *et al.* [91] and Wang and Sanders [101], ξ^2 provides a sufficient entanglement criterion for atomic ensembles. On top of that, spin squeezing parameter is particularly appreciated by experimentalists since: i) it has a clear physical meaning, ii) it can be relatively easy measured, iii) it is defined by a simple operational expression, iv) it provides a figure of merit for atomic clocks. However, until our recent works [51] and [52] no further investigations to relate ξ^2 to other concepts of quantum information have been carried out.

5.1.4 Our approach

In this Chapter we generalize and connect the concept of the spin squeezing parameter to the theory of entanglement witnesses (Definition 3.3, Section 3.1.2), i.e. such observables $\mathcal{W}$ that have non-negative averages for all separable states and there exists an entangled state ϱ such that $\mathrm{tr}\big(\varrho\mathcal{W}\big) < 0$. In order to derive the generalized spin squeezing inequalities, we introduce a general method of expressing state averages of the appropriate entanglement witnesses in terms of the total spin operators (5.3).

Our method works as follows. We begin with considering symmetric states of N qubits first, i.e. states ϱ that satisfy:

$$P\varrho P = \varrho, \tag{5.5}$$

where P is an orthogonal projector, i.e. it satisfies $P^2 = P$ and $P^\dagger = P$, onto the symmetrized product of individual qubit spaces $\mathcal{H}_s := \mathrm{Sym}(\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2)$ (Sym denotes symmetrization). The action of P on product vectors is defined as follows:

$$P|\psi_1\rangle \otimes \cdots \otimes |\psi_N\rangle := \frac{1}{N!} \sum_{\pi \in \mathfrak{S}_N} |\psi_{\pi(1)}\rangle \otimes \cdots \otimes |\psi_{\pi(N)}\rangle \tag{5.6}$$

and it prolongs to the whole Hilbert space by linearity. For symmetric states of two and three qubits, the necessary and sufficient condition for separability of is equivalent to the PPT condition for the state. For two qubits the PPT condition (Theorem 3.4, Section 3.1.2) is in fact the necessary and sufficient condition for separability of arbitrary (also non-symmetric) states; for symmetric states of three qubits this result has been shown by Eckert *et al.* in Ref. [20]. The knowledge of the necessary and sufficient separability criterion allows us to derive complete families of generalized spin squeezing inequalities, which provide necessary and sufficient conditions for 2-qubit, or genuine 3- qubit entanglement for symmetric states.

At the same time, our inequalities provide a sufficient condition for entanglement of general, i.e. not necessarily symmetric, states of N qubits[2]. The results of this Chapter imply also that, if we somewhat broaden the standard notion of spin squeezing (5.4), then for spin-j systems represented as a collection of $2j$ qubits, spin

[2]Note that macroscopic atomic ensembles may be prepared in symmetric subspace, although ultimately individual spontaneous emission acts take the system out of this subspace. Nevertheless, especially in mesoscopic systems, the symmetric component might remain significant for relatively long times.

squeezing becomes equivalent to bipartite entanglement among the qubits (Wang and Sanders [101] obtained the implication in one direction using different methods). We also derive and discuss somewhat simpler spin squeezing inequalities that provide sufficient conditions for genuine 3-qubit entanglement.

In order to show how to obtain our inequalities for concrete purposes, we present in this Chapter explicit derivations for the, so called, Dicke states (Dicke [15]), sometimes also called generalized W-states. We show step-by-step how to derive the inequalities probing genuine 2- and 3-qubit entanglement of these states.

Finally, we analyze with the obtained inequalities the output of the ion-trap experiment of Häffner *et al.* [36], confirming the presence of 2- and 3-qubit entanglement in the generated states. We also briefly describe this experiment: the experimental production and state tomography of 6-, 7-, and 8-particle W-states of trapped ions. We also show full reconstructed density matrix of the 7-qubit W-state.

5.2 Detection of bipartite entanglement

We say that a multiqubit state ϱ possesses 2-qubit entanglement if for some qubits a and b the reduced density matrix:

$$\varrho_{ab} = \mathrm{tr}_{1..\hat{a}..\hat{b}..N}\,\varrho \tag{5.7}$$

is entangled. The PPT criterion implies that ϱ_{ab} is entangled if and only if there exists a vector $|\psi\rangle$ such that:

$$\mathrm{tr}_{ab}\big(\varrho_{ab}|\psi\rangle\langle\psi|^{T_1}\big) < 0, \tag{5.8}$$

where transpose is defined with respect to the standard basis $|0\rangle, |1\rangle$, which throughout this Chapter we fix for each qubit space by the condition: $\sigma^z|0\rangle = |0\rangle$, $\sigma^z|1\rangle = -|1\rangle$. As $|\psi\rangle$ we can take any eigenvector of $\varrho_{ab}^{T_1}$ corresponding to any negative eigenvalue. Since for product $|\psi\rangle = |u\rangle \otimes |v\rangle$ it would hold: $\mathrm{tr}_{ab}\big(\varrho_{ab}|\psi\rangle\langle\psi|^{T_1}\big) = \langle \overline{u} \otimes v|\varrho_{ab}\,\overline{u} \otimes v\rangle \geq 0$, we see that $|\psi\rangle$ must be necessarily entangled. Note that the left hand side of the inequality (5.8) can be also viewed as an evaluation of a witness $\mathcal{W}_{ab} := |\psi\rangle\langle\psi|^{T_1}$ on ϱ_{ab}.

According to our general strategy, we first consider symmetric states, as then we can obtain a convenient parametrization of $|\psi\rangle$. In the 2-qubit case we can take advantage of the low dimensionality and use the explicit form of $\varrho_{ab}^{T_1}$. We have that:

$$\varrho^{T_1} = \begin{bmatrix} \epsilon_0 & \delta & \delta^* & \tau \\ \delta^* & \epsilon_1 & \varpi^* & \varsigma^* \\ \delta & \varpi & \epsilon_1 & \varsigma \\ \tau & \varsigma & \varsigma^* & \epsilon_2 \end{bmatrix}, \tag{5.9}$$

where $\epsilon_0, \epsilon_1, \epsilon_2, \tau \in \mathbb{R}$. It is easy to check that vectors of the type:

$$|\psi\rangle = \eta|00\rangle + \beta|01\rangle + \beta^*|10\rangle + \gamma|11\rangle, \quad \eta, \gamma \in \mathbb{R} \tag{5.10}$$

are preserved by ϱ^{T_1} and, since they have three independent parameters (we take them to be normalized, although it is not important for the condition (5.8)), it is possible to find a solution of the eigenvalue equation. Hence, any negative eigenvalue vector in the inequality (5.8) must be of this form. From Eq. (5.10) it follows that the matrix $[\psi]$ of coefficients of $|\psi\rangle$ is hermitian:

$$[\psi] = \left[\begin{array}{cc} \eta & \beta \\ \beta^* & \gamma \end{array} \right], \tag{5.11}$$

so that we can diagonalize it by some $\tilde{U} \in SU(2)$ (modulo $U(1)$ phase rotation):

$$[\psi] = \tilde{U}^\dagger \Delta \tilde{U}. \tag{5.12}$$

Note that due to the normalization of $|\psi\rangle$, the eigenvalue matrix Δ can be put in the following form:

$$\Delta = \left[\begin{array}{cc} \sin\frac{\varphi}{2} & 0 \\ 0 & \pm\cos\frac{\varphi}{2} \end{array} \right], \quad -\pi \leq \varphi \leq \pi. \tag{5.13}$$

Rewriting Eq. (5.11) explicitly in the basis and using Eq. (5.13), we finally obtain the following parametrization:

$$|\psi\rangle = U^* \otimes U |\psi_0\rangle\,, \quad |\psi_0\rangle := \sin\frac{\varphi}{2}|00\rangle + \cos\frac{\varphi}{2}|11\rangle\,, \tag{5.14}$$

where $U := \tilde{U}^T$, and we have fixed the overall phase. The parameters η, β, γ from the decomposition (5.10) are now encoded into φ and U. Using the above parametrization inequality (5.8) takes the following form:

$$\mathrm{tr}_{ab}\big(\varrho_{ab} U \otimes U |\psi_0\rangle\langle\psi_0|^{T_1} U^\dagger \otimes U^\dagger\big) < 0\,. \tag{5.15}$$

In order to rewrite the condition (5.15) with the total spin operators (5.3), first note that $|\psi_0\rangle\langle\psi_0|^{T_1}$ can be decomposed into Pauli matrices as follows:

$$\begin{aligned} |\psi_0\rangle\langle\psi_0|^{T_1} \;=\; & \frac{1}{4}\sin^2\frac{\varphi}{2}\big(\mathbf{1}+\sigma^z\big)\otimes\big(\mathbf{1}+\sigma^z\big) + \frac{1}{4}\cos^2\frac{\varphi}{2}\big(\mathbf{1}-\sigma^z\big)\otimes\big(\mathbf{1}-\sigma^z\big) \\ & + \frac{1}{4}\sin\varphi\big(\sigma^x\otimes\sigma^x + \sigma^y\otimes\sigma^y\big). \end{aligned} \tag{5.16}$$

Then, the adjoint action of $SU(2)$ in the inequality (5.15) induces a $SO(3)$ rotation R of the Pauli matrices: $U\sigma^i U^\dagger = R^i{}_j \sigma^j$ (the repeated indices are summed over). We will denote the axes of the rotated frame by $\mathbf{k}, \mathbf{l}, \mathbf{n}$.

Since in the symmetric case we currently consider all the reductions ϱ_{ab} are of the same form, we can sum the inequalities (5.15) over all pairs of qubits: $\sum_{\langle ab\rangle} := \sum_{a=1}^{N-1}\sum_{b=a+1}^{N}$, without affecting the inequality sign. However, before we do so, we extend the operator $|\psi\rangle\langle\psi|^{T_1}$ from the space of the qubits ab to the full Hilbert space of N qubits by: $|\psi\rangle_{ab}\langle\psi|^{T_1} := |\psi\rangle\langle\psi|^{T_1} \otimes \mathbf{1}_{1..\hat{a}..\hat{b}..N}$. Then, we obtain that:

$$\sum_{\langle ab\rangle} \mathrm{tr}_{ab}\big(\varrho_{ab}|\psi\rangle\langle\psi|^{T_1}\big) = \mathrm{tr}\big(\varrho \sum_{\langle ab\rangle} |\psi\rangle_{ab}\langle\psi|^{T_1}\big). \tag{5.17}$$

Now we can plug the Pauli matrix decomposition (5.16) into Eq. (5.17), and, using the identity:

$$\sum_{\langle ab\rangle} \sigma_a^i \otimes \sigma_b^i = 2(J^i)^2 - \frac{N}{2}, \tag{5.18}$$

(coming directly from the definition of $\mathbf{J}$ (5.3)) obtain the desired form of the condition (5.8): a symmetric state ϱ possesses bipartite entanglement if and only if there exist $-\pi \leq \varphi \leq \pi$ and $U \in SU(2)/U(1)$, such that the following inequality holds:

$$\begin{aligned} \sin\varphi\Big[\langle J_{\mathbf{k}}^2\rangle + \langle J_{\mathbf{l}}^2\rangle - \frac{N}{2}\Big] - (N-1)\cos\varphi\,\langle J_{\mathbf{n}}\rangle \\ + \langle J_{\mathbf{n}}^2\rangle + \frac{N(N-2)}{4} < 0, \end{aligned} \tag{5.19}$$

where all the averages are taken with respect to the full N-qubit state ϱ.

Note that alternatively sums like Eq. (5.17) can be calculated using the spin-coherent P-representation of ϱ_{ab} (Eq. (3.20), Section 3.2). Since ϱ_{ab} is symmetric, it of the form:

$$\varrho_{ab} = \int_{\mathbb{S}^2} \mathrm{d}\Omega\, P_\varrho(\theta,\varphi)\, |\theta,\varphi\rangle\langle\theta,\varphi| \otimes |\theta,\varphi\rangle\langle\theta,\varphi|, \tag{5.20}$$

where the spin-coherent states $|\theta,\varphi\rangle$ for qubits, i.e. for the fundamental representation of $SU(2)$, are given by a simple expression:

$$|\theta,\varphi\rangle = \cos\frac{\theta}{2}\,|0\rangle + \mathrm{e}^{\mathrm{i}\varphi}\sin\frac{\theta}{2}\,|1\rangle, \tag{5.21}$$

and every pure qubit state is representable in this form. The above observation connects the approach of this Chapter to the various characteristic functions methods of the preceding Chapters.

In case of a general, i.e. not necessarily symmetric, state ϱ observe that, if there exist $-\pi \leq \varphi \leq \pi$ and $U \in SU(2)/U(1)$ the same for all pairs of qubits, and such that the sum (5.17) is negative, then there must be at least one pair of qubits ab for which $\mathrm{tr}_{ab}\big(\varrho_{ab}|\psi\rangle\langle\psi|^{T_1}\big) < 0$, and hence the state ϱ possesses bipartite entanglement. Thus, the condition (5.19) is also a sufficient condition for bipartite entanglement for general states.

For a given negative eigenvalue vector $|\psi\rangle$ the left hand side of the inequality (5.19) is completely determined. However, we can also treat it as a function of the parameters of $|\psi\rangle$, and as such it can be optimized. In particular, keeping the frame $\mathbf{k},\mathbf{l},\mathbf{n}$ fixed, we can search for the minimum with respect to the angle φ. Let us call this minimum φ_0. Clearly, if the inequality (5.19) is satisfied for some φ, then it will be also satisfied for φ_0, and vice versa. Hence, it is enough to check the condition (5.19) only for φ_0. Performing the minimization, we obtain that:

$$\sin\varphi_0 = -\frac{\langle J_{\mathbf{k}}^2\rangle + \langle J_{\mathbf{l}}^2\rangle - N/2}{\sqrt{\big[\langle J_{\mathbf{k}}^2\rangle + \langle J_{\mathbf{l}}^2\rangle - N/2\big]^2 + (N-1)^2\langle J_{\mathbf{n}}\rangle^2}}, \tag{5.22}$$

$$\cos\varphi_0 = \frac{(N-1)\langle J_{\mathbf{n}}\rangle}{\sqrt{\big[\langle J_{\mathbf{k}}^2\rangle + \langle J_{\mathbf{l}}^2\rangle - N/2\big]^2 + (N-1)^2\langle J_{\mathbf{n}}\rangle^2}}, \tag{5.23}$$

and the inequality (5.19) becomes:

$$\langle J_{\mathbf{n}}^2\rangle + \frac{N(N-2)}{4} < \sqrt{\left[\langle J_{\mathbf{k}}^2\rangle + \langle J_{\mathbf{l}}^2\rangle - \frac{N}{2}\right]^2 + (N-1)^2\langle J_{\mathbf{n}}\rangle^2}\,. \tag{5.24}$$

As a result, we arrive at the following Theorem:

Theorem 5.1 (Criterion for bipartite entanglement). *If there exist mutually orthogonal directions* $\mathbf{k}$, $\mathbf{l}$, $\mathbf{n}$ *such that the inequality (5.24) holds, then the state* ϱ *possesses bipartite entanglement. For symmetric states the above condition is both necessary and sufficient.*

In the latter case, due to the equality:

$$\langle J_{\mathbf{k}}^2\rangle + \langle J_{\mathbf{l}}^2\rangle + \langle J_{\mathbf{n}}^2\rangle = \frac{N(N+2)}{4}, \tag{5.25}$$

the criterion (5.24) can be simplified to:

$$\frac{4\langle \Delta J_{\mathbf{n}}^2\rangle}{N} < 1 - \frac{4\langle J_{\mathbf{n}}\rangle^2}{N^2}. \tag{5.26}$$

The relation of the criterion (5.24) to the standard spin squeezing condition (5.4) is the following. Spin-j state can be equivalently represented as a symmetric state of $N = 2j$ qubits. Intuitively, spin squeezing should refer to existence of non-classical correlations among the qubits, as argued by Kitagawa and Ueda [46]. Indeed, criterion (5.26) provides a rigorous proof for this intuitive picture, as, on one hand, if the condition (5.4) is satisfied, then the inequality (5.26) is satisfied as well, since in this particular case $\langle J_{\mathbf{n}}\rangle = 0$ and $j = N/2$. Hence, spin-j squeezed states possess 2-qubit entanglement (Wang and Sanders [101]). On the other hand, if we broaden the standard definition of spin squeezing (Definition 5.2), and allow the direction $\mathbf{n}$ to be arbitrary, then we also obtain the converse statement: the condition (5.26) implies existence of a spin component $J_{\mathbf{n}}$, such that $\langle \Delta J_{\mathbf{n}}^2\rangle < j/2$. Note however that from the condition (5.26) it does not follow that the direction of squeezing $\mathbf{n}$ is orthogonal to $\langle \mathbf{J}\rangle$. Thus, we obtain a more general type of squeezing. In Section 5.5 we will show somewhat extreme examples of state, for which $\mathbf{n}$ is actually parallel to the mean spin.

5.3 Detection of tripartite entanglement

As in the previous Section, we begin with considering symmetric states first. The PPT criterion still works for the tripartite reductions ϱ_{abc} of such states, since $\mathrm{Sym}(\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2)$ is a subspace of $\mathbb{C}^2\otimes\mathrm{Sym}(\mathbb{C}^2\otimes\mathbb{C}^2) = \mathbb{C}^2\otimes\mathbb{C}^3$. Thus, we can proceed as before.

From the above identification and the remark after the inequality (5.8), vector $|\psi\rangle$, corresponding to any negative eigenvalue of $\varrho_{abc}^{T_1}$ must be necessarily a 3-party entangled vector from $\mathbb{C}^2\otimes\mathrm{Sym}(\mathbb{C}^2\otimes\mathbb{C}^2)$. As we mentioned in Section 5.1.1, the

parametrization of such vectors was found by Dür *et al.* in Ref. [19]; there are two families:

$$|\psi\rangle = A \otimes B \otimes B |GHZ_3\rangle, \tag{5.27}$$

$$|\psi\rangle = A \otimes U \otimes U |W_3\rangle\,. \tag{5.28}$$

Here, matrices $A, B \in SL(2,\mathbb{C})$, $U \in SU(2)$, and vectors $|GHZ_3\rangle$ and $|W_3\rangle$ are given by Eqs. (5.2) and (5.1) respectively. The action of $SL(2,\mathbb{C})$ on the Pauli matrices in the decomposition of $|\psi\rangle\langle\psi|^{T_1}$ now induces restricted, i.e. orientation and time-orientation preserving, Lorenz transformations:

$$A^* \sigma^\mu A^T = \Lambda^\mu{}_\nu \sigma^\nu\,,\ B \sigma^\mu B^\dagger = L^\mu{}_\nu \sigma^\nu\,,\ \sigma^0 := \mathbf{1} \tag{5.29}$$

(Greek indices run through $0 \ldots 3$), and the PPT condition takes the following form:

$$\mathrm{tr}_{abc}\big(\varrho_{abc} |\psi\rangle\langle\psi|^{T_1}\big) = \tfrac{1}{8} K_{\alpha\beta\gamma} \mathrm{tr}_{abc}\big(\varrho_{abc} \sigma^\alpha \otimes \sigma^\beta \otimes \sigma^\gamma\big) < 0 \tag{5.30}$$

(note the summation convention). Tensor $K_{\alpha\beta\gamma}$ is introduced for compactness of the notation. It is read off directly from the decomposition of $|GHZ_3\rangle\langle GHZ_3|^{T_1}$ and $|W_3\rangle\langle W_3|^{T_1}$ into Pauli matrices. For the GHZ-family (5.27) it is equal to:

$$\begin{aligned} K_{\alpha\beta\gamma}(\Lambda, L) \;=\; & \Lambda^0{}_\alpha L^0{}_\beta L^0{}_\gamma + \Lambda^0{}_\alpha L^3{}_\beta L^3{}_\gamma + \Lambda^1{}_\alpha L^1{}_\beta L^1{}_\gamma + 2\Lambda^3{}_\alpha L^0{}_{(\beta} L^3{}_{\gamma)} \\ & - \Lambda^1{}_\alpha L^2{}_\beta L^2{}_\gamma + 2\Lambda^2{}_\alpha L^1{}_{(\beta} L^2{}_{\gamma)}\,, \end{aligned} \tag{5.31}$$

while for the W-family (5.28) it reads:

$$\begin{aligned} K_{\alpha\beta\gamma}(\Lambda, R) \;=\; & \frac{1}{3}\Big\{ 3\Lambda^0{}_\alpha R^0{}_\beta R^0{}_\gamma - 3\Lambda^3{}_\alpha R^3{}_\beta R^3{}_\gamma + 2\Lambda^0{}_\alpha R^0{}_{(\beta} R^3{}_{\gamma)} \\ & + \Lambda^3{}_\alpha R^0{}_\beta R^0{}_\gamma - \Lambda^0{}_\alpha R^3{}_\beta R^3{}_\gamma - 2\Lambda^3{}_\alpha R^0{}_{(\beta} R^3{}_{\gamma)} \\ & + 4\Lambda^1{}_\alpha R^0{}_{(\beta} R^1{}_{\gamma)} + 4\Lambda^1{}_\alpha R^1{}_{(\beta} R^3{}_{\gamma)} - 4\Lambda^2{}_\alpha R^0{}_{(\beta} R^2{}_{\gamma)} \\ & - 4\Lambda^2{}_\alpha R^2{}_{(\beta} R^3{}_{\gamma)} + 2\Lambda^0{}_\alpha R^1{}_\beta R^1{}_\gamma + 2\Lambda^3{}_\alpha R^1{}_\beta R^1{}_\gamma \\ & + 2\Lambda^3{}_\alpha R^2{}_\beta R^2{}_\gamma + 2\Lambda^0{}_\alpha R^2{}_\beta R^2{}_\gamma \Big\}\,. \end{aligned} \tag{5.32}$$

Here, $R^\mu{}_\nu$ is the natural four-dimensional embedding of the rotation generated by U from Eq. (5.28), and the round brackets ( ) around indices denote symmetrization, e.g. $A^{(\mu\nu)} := (A^{\mu\nu} + A^{\nu\mu})/2$. Note that the relativistic notation is used only for our convenience. We could have as well put all the indices at the same level as we are *n*ot going to lower or rise them with the Minkowski metric.

Next, we sum the inequalities (5.30) over all possible triples of qubits: $\sum_{\langle abc\rangle} := \sum_{a=1}^{N-2} \sum_{b=a+1}^{N-1} \sum_{c=b+1}^{N}$, just like we summed the inequalities (5.15) in the previous Section:

$$\sum_{\langle abc\rangle} K_{\alpha\beta\gamma} \mathrm{tr}_{abc}\big(\varrho_{abc} \sigma^\alpha \otimes \sigma^\beta \otimes \sigma^\gamma\big) = K_{\alpha\beta\gamma} \mathrm{tr}\Big(\varrho \sum_{\langle abc\rangle} \sigma_a^\alpha \otimes \sigma_b^\beta \otimes \sigma_c^\gamma\Big). \tag{5.33}$$

Because of the symmetry condition (5.5), we can rewrite Eq. (5.33) as follows:

$$K_{\alpha\beta\gamma} \mathrm{tr}\big(\varrho P \sum_{\langle abc\rangle} \sigma_a^\alpha \otimes \sigma_b^\beta \otimes \sigma_c^\gamma P\big), \tag{5.34}$$

and observe that due to the action of P, we can substitute $\sigma_a^\alpha \otimes \sigma_b^\beta \otimes \sigma_c^\gamma$ with the symmetrized product: $\sigma_a^{(\alpha} \otimes \sigma_b^\beta \otimes \sigma_c^{\gamma)}$. This finally allows us to rewrite Eq. (5.34) with the total spin operators J^i (supplemented by an artificial "time-component" $J^0 = (N/2)\mathbf{1}$ for compactness of the notation), thanks to the identity:

$$\begin{aligned} 3\sum_{\langle abc\rangle} \sigma_a^{(\alpha} \otimes \sigma_b^\beta \otimes \sigma_c^{\gamma)} &= 4J^{(\alpha}J^\beta J^{\gamma)} - 6f^{(\alpha\beta}{}_\mu J^{(\gamma}J^{\mu)} + 2f^{(\alpha\beta}{}_\mu f^{(\gamma)\mu)}{}_\nu J^\nu \\ &\quad - f^{(\alpha\beta}{}_\mu f^{[\gamma)\mu]}{}_\nu J^\nu \,. \end{aligned} \tag{5.35}$$

The symmetrization above is taken with respect to $\alpha\beta\gamma$ and $\gamma\mu$ separately and the square brackets [ ] around Greek indices denote antisymmetrization, e.g. $A^{[\mu\nu]} := (A^{\mu\nu} - A^{\nu\mu})/2$. The constants $f^{\alpha\beta}{}_\gamma$ are defined through: $\sigma^\mu\sigma^\nu =: f^{\mu\nu}{}_\gamma\sigma^\gamma$. Their numerical values are as follows:

$$f^{0\alpha}{}_\beta = f^{\alpha 0}{}_\beta = \delta^\alpha{}_\beta, \quad f^{ij}{}_\alpha = \mathrm{i}\sum_l \epsilon^{ijl}\delta^l{}_\alpha + \delta^{ij}\delta^0{}_\alpha. \tag{5.36}$$

Substituting Eq. (5.35) into Eq. (5.34) leads us to the following criterion

Theorem 5.2 (Criterion for tripartite entanglement). *A symmetric state ϱ possesses genuine tripartite entanglement if and only if there exist two restricted Lorenz transformations Λ, L, or a restricted Lorenz transformation Λ and a rotation R, such that:*

$$\begin{aligned} X(\varrho) &:= K_{(\alpha\beta\gamma)}\Big\{2\langle J^\alpha J^\beta J^\gamma\rangle - 3f^{\alpha\beta}{}_\mu\langle J^{(\gamma}J^{\mu)}\rangle + f^{\alpha\beta}{}_\mu f^{(\gamma\mu)}{}_\nu\langle J^\nu\rangle \\ &\quad - \frac{1}{2}f^{\alpha\beta}{}_\mu f^{[\gamma\mu]}{}_\nu\langle J^\nu\rangle\Big\} < 0 \end{aligned} \tag{5.37}$$

holds, with $K_{\alpha\beta\gamma}$ given by Eq. (5.31), or by Eq. (5.32) respectively.

The above criterion detects genuine tripartite entanglement (see Definition 5.1), because as due to the symmetry condition (5.5) there are no biseparable symmetric states.

For a general state ϱ we could, as in the previous Section, generate a sufficient entanglement condition by applying the same witness $|\psi\rangle\langle\psi|^{T_1}$, with $|\psi\rangle$ given by Eq. (5.27) or by Eq. (5.28), to all tripartite reductions ϱ_{abc}. However, then we cannot use the symmetry arguments like we used in Eq. (5.34), and directly apply the identity (5.35). Instead, we construct from the families (5.27) and (5.28) different witnesses, given for the W-family (5.28) by:

$$\begin{aligned} &\frac{1}{3}\Big\{\big(A\otimes U\otimes U|W_3\rangle\langle W_3|A^\dagger\otimes U^\dagger\otimes U^\dagger\big)^{T_1} \\ &+\big(U\otimes A\otimes U|W_3\rangle\langle W_3|U^\dagger\otimes A^\dagger\otimes U^\dagger\big)^{T_2} \\ &+\big(U\otimes U\otimes A|W_3\rangle\langle W_3|U^\dagger\otimes U^\dagger\otimes A^\dagger\big)^{T_3}\Big\}, \end{aligned} \tag{5.38}$$

and analogously for the GHZ-family (5.27). We then apply the witnesses (5.38) to all tripartite reductions of ϱ, which effectively leads to the substitution of $K_{\alpha\beta\gamma}$

by $K_{(\alpha\beta\gamma)}$ in Eq. (5.33)[3]. Hence, we can use Eq. (5.35) again and arrive at the condition (5.37).

The price to pay, apart from the mere sufficiency of the condition (5.37), is that the witnesses (5.38) make no distinction between biseparable tripartite reductions (which are now not forbidden by the symmetry) and genuine 3-qubit entangled ones, and hence, the inequality (5.37) indicates only general 3-qubit entanglement. However, note that the set of all biseparable states is closed, and hence each genuine 3-qubit entangled state possesses an open neighbourhood consisting of only genuine 3-qubit entangled states. Thus, the criterion (5.37) also detects genuine 3-qubit entangled states in some open vicinity of symmetric states, but the size of this vicinity is a priori not known (the same remark applies to the criterion (5.26) as well). We will partially solve this drawback using another witnesses in Section 5.7.

5.4 Full separability

There is a connection between full, i.e. N-qubit, separability of symmetric states and the classicality problem, we discussed in Chapter 2. Consider the spin-coherent P-representation of a symmetric state:

$$\varrho = \int_{\mathbb{S}^2} \mathrm{d}\Omega\, P_\varrho(\theta,\varphi)\, |\theta,\varphi\rangle\langle\theta,\varphi| \otimes \cdots \otimes |\theta,\varphi\rangle\langle\theta,\varphi|. \tag{5.39}$$

As we mentioned at the end of Section 3.2, the representation (5.39) is not unique, because in the decomposition of $P_\varrho(\theta,\varphi)$ over the spherical harmonics Y_{lm}, ϱ determines only terms with[4] $l \leq N$. Hermiticity and normalization of ϱ implies that $\overline{P_\varrho(\theta,\varphi)} = P_\varrho(\theta,\varphi)$ and $\int \mathrm{d}\Omega\, P_\varrho(\theta,\varphi) = 1$, while positivity imposes further constraints, which is satisfied e.g. by probabilistic measures on the sphere. However, just like in the case of the standard P-representation, the space of allowed $P_\varrho(\theta,\varphi)$'s is larger than that and the following fact holds (Braunstein *et al.* [10], Kraus [56]):

Proposition 5.1. *A symmetric state ϱ is fully separable if and only if there exists a representation (5.39) where $P_\varrho(\theta,\varphi)d\Omega$ is an element of a probabilistic measure on $\mathbb{S}^2$.*

Proof. The implication in one direction is obvious, as the integral in (5.39) is a norm limit of separable states. To prove the implication in the other direction, observe that if ϱ is separable, then it can be decomposed as follows: $\varrho = \sum_i p_i |\theta_i,\varphi_i\rangle\langle\theta_i,\varphi_i| \otimes \cdots \otimes |\theta_i,\varphi_i\rangle\langle\theta_i,\varphi_i|$, $p_i \geq 0$, $\sum p_i = 1$, since vectors of the form $|\theta_i,\varphi_i\rangle\langle\theta_i,\varphi_i| \otimes \cdots \otimes |\theta_i,\varphi_i\rangle\langle\theta_i,\varphi_i|$ are the only symmetric product vectors. We define then $P_\varrho(\theta,\varphi) := \sum_i p_i \delta(\cos\theta - \cos\theta_i)\delta(\varphi - \varphi_i)$; the expansion of δ's over Y_{lm} can be truncated at $l = N$. □

[3] Note that the witnesses (5.38) are not equal to $P|\psi\rangle\langle\psi|^{T_1}P$, which would merely lead to cutting the symmetric part from ϱ.

[4] We can fix this freedom by setting to zero all higher-order terms; functions $P_\varrho(\theta,\varphi)$ are then at most Nth order polynomials in the Cartesian coordinates on the sphere.

Note the similarity between the above Proposition and Definition 2.1 of the classicality of a state of a mechanical system. Next, observe that if $\mathcal{W}$ is an entanglement witness, then:

$$\mathrm{tr}\big(\varrho\mathcal{W}\big) = \int \mathrm{d}\Omega\, P_\varrho(\theta,\varphi)\, w(\theta,\varphi) \tag{5.40}$$

where:

$$w(\theta,\varphi) := \langle(\theta,\varphi)^{\otimes N}|\mathcal{W}\,(\theta,\varphi)^{\otimes N}\rangle \tag{5.41}$$

is a Nth order positive semidefinite (since $\mathcal{W}$ is non-negative on separable states) polynomial in the Cartesian coordinates:

$$x := \langle\theta,\varphi|\sigma^x|\theta,\varphi\rangle, \quad y := \langle\theta,\varphi|\sigma^y|\theta,\varphi\rangle, \quad z := \langle\theta,\varphi|\sigma^z|\theta,\varphi\rangle. \tag{5.42}$$

Hence, ϱ is entangled if and only if there exists a polynomial $w(x,y,z)$, which is PSD on $\mathbb{S}^2$ and for which the integral (5.40) is negative. The above fact establishes an interesting link between the separability of symmetric states of N qubits and the polynomial non-classicality witnesses from Theorem 2.4 from Section 2.4. The criteria (5.26) and (5.37), with the reversed inequality signs, can be thus interpreted as the necessary and sufficient conditions for $P_\varrho(\theta,\varphi)\mathrm{d}\Omega$ to be an element of a probabilistic measure on $\mathbb{S}^2$ in the order $N=2$ and $N=3$ in the spherical harmonics.

5.5 An example - Dicke states

In this Section we apply our methods to the theoretical study of the family of Dicke states (Dicke [15]):

$$|\Psi_{N,k}\rangle := \binom{N}{k}^{-\frac{1}{2}} \big(|\underbrace{11\ldots1}_{k}000\ldots0\rangle + \mathrm{perm}\big)\,, \tag{5.43}$$

('perm' stands for all possible remaining permutations), which are generalizations of N-qubit W-states $|W_N\rangle$:

$$|W_N\rangle = |\Psi_{N,1}\rangle. \tag{5.44}$$

We explicitly construct for $|\Psi_{N,k}\rangle$ the inequalities (5.24) and (5.37). In particular, we derive all the necessary expressions for the analysis of the experimental data on 7- and 8-qubit W-states, which we will perform in the next Section.

For practical reasons, we choose the number of excited qubits k to be smaller than the integer part of $N/2$. Also note that alternatively the states (5.43) can be defined as the eigenstates of the total angular momentum:

$$|\Psi_{N,k}\rangle = |N/2, N/2-k\rangle. \tag{5.45}$$

We first consider 2-qubit entanglement. All the reduced 2-qubit density matrices have the same form:

$$\varrho_2 = \binom{N}{k}^{-1} \Big(c_0|00\rangle\langle 00| + c_1|11\rangle\langle 11| + 2c_+|\Psi_+\rangle\langle\Psi_+|\Big)\,, \tag{5.46}$$

where $|\Psi_+\rangle = 1/\sqrt{2}(|01\rangle + |10\rangle)$ is one of the Bell basis states (c.f. Eq. (6.22)) and the coefficients are given by the following binomials:

$$c_0 := \binom{N-2}{k}, \quad c_1 := \binom{N-2}{k-2}, \quad c_+ := \binom{N-2}{k-1}. \tag{5.47}$$

The partially transposed matrix $\varrho_2^{T_1}$ in the basis $|00\rangle, |11\rangle, |01\rangle, |10\rangle$ is given by:

$$\varrho_2^{T_1} = \binom{N}{k}^{-1} \begin{pmatrix} c_0 & c_+ & 0 & 0 \\ c_+ & c_1 & 0 & 0 \\ 0 & 0 & c_+ & 0 \\ 0 & 0 & 0 & c_+ \end{pmatrix}. \tag{5.48}$$

In the generic case, when all the constants from Eqs. (5.47) are non-zero, $\varrho_2^{T_1}$ has one negative eigenvalue:

$$\lambda_- = \frac{1}{2}\binom{N}{k}^{-1}\big(c_0 + c_1 - \sqrt{(c_0 - c_1)^2 + 4c_+^2}\big), \tag{5.49}$$

as $c_0 c_1 - c_+^2 < 0$, and hence the states (5.43) possess bipartite entanglement. The normalized eigenvector corresponding to λ_- is given by:

$$|\psi\rangle = \frac{1}{\sqrt{1+t^2}}\big(|00\rangle - t|11\rangle\big), \tag{5.50}$$

$$t := \frac{c_0 - c_1}{2c_+} + \sqrt{\Big(\frac{c_0 - c_1}{2c_+}\Big)^2 + 1}\,. \tag{5.51}$$

We see that $|\psi\rangle$ is already in the form $|\psi_0\rangle$ from Eq. (5.14) with respect to the chosen basis, and hence no unitary rotation U is needed. As that rotation was the only ingredient needed to construct the spin squeezing inequalities (5.24) and (5.26) (because the angle φ is minimized over), we simply put $\mathbf{k}, \mathbf{l}, \mathbf{n} = x, y, z$ in them.

Although in theory both inequalities (5.24) and (5.26) are equivalent, and we could use the latter due to simplicity, the inequality to be measured is rather (5.24) as in real-life experiments one does not obtain perfectly symmetric states. Using Eq. (5.45) we find that for the perfect Dicke states:

$$\langle (J^z)^2\rangle + \frac{N(N-2)}{4} = \frac{N(N-1)}{2} - Nk + k^2, \tag{5.52}$$

$$\sqrt{\Big[\langle (J^x)^2\rangle + \langle (J^y)^2\rangle - \frac{N}{2}\Big]^2 + (N-1)^2\langle J^z\rangle^2} = \sqrt{(Nk - k^2)^2 + \frac{(N-1)^2(N-2k)^2}{4}}. \tag{5.53}$$

For the experimentally interesting examples of the 7- and 8-qubit W-states $|W_7\rangle$, $|W_8\rangle$, the expressions (5.52) and (5.53) take the following values: 15.000 and 16.155 respectively for $|W_7\rangle$; 21.000 and 22.136 respectively for $|W_8\rangle$.

Let us now proceed with the analysis of tripartite entanglement. All the tripartite reductions are of the form:

$$\varrho_3 = \binom{N}{k}^{-1}\Big(\kappa_0|000\rangle\langle 000| + \kappa_1|111\rangle\langle 111| + 3\omega|W_3\rangle\langle W_3| + 3\omega'|W_3'\rangle\langle W_3'|\Big), \tag{5.54}$$

where $|W_3'\rangle := 1/\sqrt{3}\,(|011\rangle + |101\rangle + |110\rangle)$, and

$$\kappa_0 := \binom{N-3}{k}, \quad \kappa_1 := \binom{N-3}{k-3}, \tag{5.55}$$

$$\omega := \binom{N-3}{k-1}, \quad \omega' := \binom{N-3}{k-2}. \tag{5.56}$$

In the basis $|000\rangle, |110\rangle, |101\rangle, |010\rangle, |001\rangle, |111\rangle, |100\rangle, |011\rangle$ the partially transposed matrix $\varrho_3^{T_1}$ reads:

$$\varrho_3^{T_1} = \binom{N}{k}^{-1}\begin{pmatrix} \kappa_0 & \omega & \omega & 0 & 0 & 0 & 0 & 0 \\ \omega & \omega' & \omega' & 0 & 0 & 0 & 0 & 0 \\ \omega & \omega' & \omega' & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \omega & \omega & \omega' & 0 & 0 \\ 0 & 0 & 0 & \omega & \omega & \omega' & 0 & 0 \\ 0 & 0 & 0 & \omega' & \omega' & \kappa_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \omega & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \omega' \end{pmatrix}. \tag{5.57}$$

In a generic case it has two negative eigenvalues:

$$\mu_- = \frac{1}{2}\binom{N}{k}^{-1}\big(\kappa_0 + 2\omega' - \sqrt{(\kappa_0 - 2\omega')^2 + 8\omega^2}\big), \tag{5.58}$$

$$\mu_-' = \frac{1}{2}\binom{N}{k}^{-1}\big(\kappa_1 + 2\omega - \sqrt{(\kappa_1 - 2\omega)^2 + 8\omega'^2}\big) \tag{5.59}$$

(because $\kappa_0\omega' < \omega^2$ and $\kappa_1\omega < \omega'^2$), and thus the states $|\Psi_{N,k}\rangle$ possess tripartite entanglement as well. Since there are two generically different negative eigenvalues, there will be two different spin squeezing inequalities (5.37). As before, we will generate them from the corresponding eigenvectors, which read:

$$|\psi\rangle = |000\rangle - \alpha|1\rangle \otimes \big(|01\rangle + |10\rangle\big), \tag{5.60}$$

$$|\psi'\rangle = |111\rangle - \alpha'|0\rangle \otimes \big(|01\rangle + |10\rangle\big), \tag{5.61}$$

where:

$$\alpha := \frac{\kappa_0 - 2\omega'}{4\omega} + \sqrt{\Big(\frac{\kappa_0 - 2\omega'}{4\omega}\Big)^2 + \frac{1}{2}}, \tag{5.62}$$

$$\alpha' := \frac{\kappa_1 - 2\omega}{4\omega'} + \sqrt{\Big(\frac{\kappa_1 - 2\omega}{4\omega'}\Big)^2 + \frac{1}{2}}. \tag{5.63}$$

Note that the vectors (5.60), (5.61) are not normalized, as the norm2 is irrelevant for the PPT condition (5.30). After proper rescaling, $|\psi\rangle$ and $|\psi'\rangle$ can be rewritten in the desired form (5.28):

$$|\psi\rangle = A \otimes \mathbf{1} \otimes \mathbf{1}|W_3\rangle, \tag{5.64}$$
$$|\psi'\rangle = A' \otimes \sigma^x \otimes \sigma^x|W_3\rangle, \tag{5.65}$$

where $A, A' \in SL(2,\mathbb{C})$ are defined as follows:

$$A := \pm \begin{pmatrix} 0 & \frac{1}{\sqrt{\alpha}} \\ -\sqrt{\alpha} & 0 \end{pmatrix}, \tag{5.66}$$

$$A' := \pm \begin{pmatrix} \mathrm{i}\sqrt{\alpha'} & 0 \\ 0 & -\frac{\mathrm{i}}{\sqrt{\alpha'}} \end{pmatrix}. \tag{5.67}$$

Before we proceed with the construction of the inequalities (5.37), let us note that having the *explicit* forms of the negative eigenvalues and the corresponding eigenvectors of $\varrho_3^{T_1}$, it is straightforward to calculate the sum over all triples of qubits (5.30). It is just given by:

$$\begin{aligned} \sum_{\langle abc \rangle} \mathrm{tr}_{abc}\big(\varrho_{abc}|\psi\rangle\langle\psi|^{T_1}\big) &= \binom{N}{3}\mu_-||\psi||^2 \\ &= \binom{N}{3}\mu_- \frac{2\alpha^2+1}{3\alpha}, \end{aligned} \tag{5.68}$$

for μ_- and $|\psi\rangle$, and by the analogous expression for μ'_- and $|\psi'\rangle$. However, our goal here is to express Eq. (5.68) using total angular momentum, in order to make it experimentally available and connect it with the spin squeezing.

Hence, following the procedure described in Section 5.3, we first have to find the Lorenz transformations and rotations generated by matrices A and A' from Eqs. (5.64) and (5.65). These transformations are the following: matrix (5.66) generates, according to Eq. (5.29), a rotation by π around y-axis, followed by a boost along z-axis:

$$\Lambda(A) = \begin{pmatrix} \gamma & 0 & 0 & -\gamma\beta \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \gamma\beta & 0 & 0 & -\gamma \end{pmatrix}, \tag{5.69}$$

$$\beta := \frac{\alpha^2-1}{\alpha^2+1}, \gamma := \frac{1}{\sqrt{1-\beta^2}}. \tag{5.70}$$

Obviously the identity operator $\mathbf{1}$ from Eq. (5.64) generates the trivial rotation, so we have in this case $R = \mathbf{1}$. Matrix (5.67) generates the rotation by π around z-axis,

followed by a boost along it:

$$\Lambda(A') = \begin{pmatrix} \gamma' & 0 & 0 & \gamma'\beta' \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \gamma'\beta' & 0 & 0 & \gamma' \end{pmatrix}, \tag{5.71}$$

$$\beta' := \frac{\alpha'^2 - 1}{\alpha'^2 + 1}, \gamma' := \frac{1}{\sqrt{1-\beta'^2}}, \tag{5.72}$$

while σ^x from Eq. (5.65) generates rotations by π around x-axis:

$$R(\sigma^x) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{5.73}$$

in the spaces of the second and the third qubit.

Next, from the matrices $\Lambda(A)$, $R = \mathbf{1}$, and $\Lambda(A')$, $R(\sigma^x)$, we build two copies of the tensor $K_{\alpha\beta\gamma}$, according to Eq. (5.32). Finally, having $K_{\alpha\beta\gamma}$, we construct the corresponding parameters $X(\Psi_{N,k})$, defined in Eq. (5.37), and check the 3-qubit spin squeezing inequalities. The resulting expressions are lengthy but straightforward, and hence we will omit them here. Let us stress that for the ideal, generic Dicke states we obtain two independent inequalities, and both of them must be satisfied. Fig. 5.1 shows the plots[5] of $X(\Psi_{N,k})$ as a function of N and k.

Let us now analyze the N-qubit W-states $|W_N\rangle$ of Eq. (5.44). In this case, from Eqs. (5.55) and (5.56) we see that $\kappa_0 = N-3$, $\omega = 1$, and $\kappa_1 = \omega' = 0$. Substituting this constants into Eqs. (5.58) and (5.59), we obtain that there remains only one negative eigenvalue of $\varrho_3^{T_1}$ given by μ_-. As a consequence, states $|W_N\rangle$ lead to only one spin squeezing inequality, generated by the matrix $\Lambda(A)$ from Eq. (5.69) and the trivial rotation $R = \mathbf{1}$. The parameter α from Eq. (5.70) is now equal to:

$$\alpha = \frac{N-3}{4} + \sqrt{\Big(\frac{N-3}{4}\Big)^2 + \frac{1}{2}}. \tag{5.74}$$

For the state $|W_7\rangle$ we obtain from the corresponding formulas that:

$$\Lambda(A) = \begin{pmatrix} 1.337 & 0 & 0 & -0.888 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0.888 & 0 & 0 & -1.337 \end{pmatrix} \tag{5.75}$$

and $X(W_7) = -44.04$.

[5]The values on the plot in Fig. 5.1 differ by the factor 12 with respect to Eq. (5.68), as we have omitted it when going from Eq. (5.30) to Eq. (5.37).

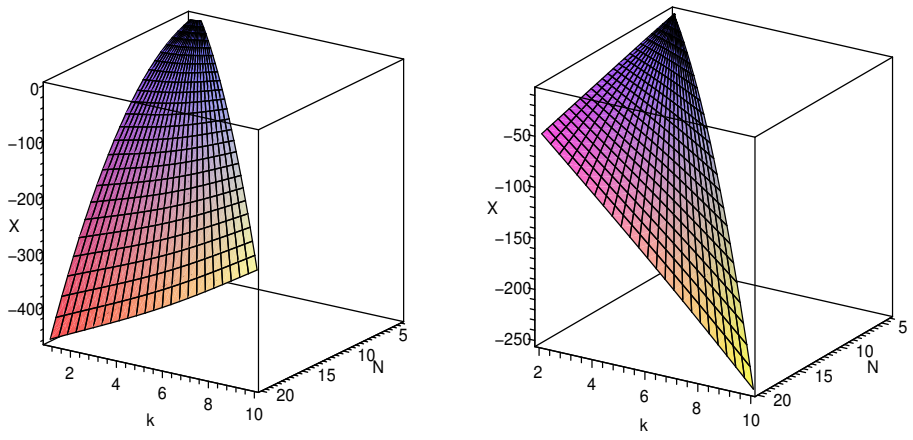

Figure 5.1: The (interpolated) plots of the parameter $X(\Psi_{N,k})$, defined in Eq. (5.37), corresponding to the eigenvectors $|\psi\rangle$ (left) and $|\psi'\rangle$ (right).

For the state $|W_8\rangle$, the corresponding matrix is given by:

$$\Lambda(A) = \begin{pmatrix} 1.529 & 0 & 0 & -1.157 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1.157 & 0 & 0 & -1.529 \end{pmatrix}. \tag{5.76}$$

and the parameter $X(W_8) = -59.88$.

To better understand the meaning of the above values of the parameter $X(\Psi_{N,k})$, let us briefly consider a less idealized situation and mix Dicke states (5.43) with the white noise:

$$\varrho_p := p|\Psi_{N,k}\rangle\langle\Psi_{N,k}| + (1-p)\frac{\mathbf{1}}{2^N}. \tag{5.77}$$

We then calculate the parameter $X(\varrho_p)$ as if the state (5.77) were an experimental output, i.e. we calculate the averages of the spin operators in Eq. (5.37) using the density matrix (5.77), while plugging the tensor $K_{\alpha\beta\gamma}$ calculated for the ideal Dicke states. Thus, we have that:

$$X(\varrho_p) = p\,X(\Psi_{N,k}) + (1-p)\,X(\mathbf{1}/2^N). \tag{5.78}$$

The results for the states $|W_7\rangle$ and $|W_8\rangle$ are presented in Fig. 5.2.

5.6 Experimental results

Let us now apply the tools developed in the previous Section to the recent experiment of Häffner *et al.* [36]. In this experiment, 7- and 8-qubit W-states have been produced in an ion trap, dedicated to quantum information processing (Schmidt-Kaler *et al.* [88]).

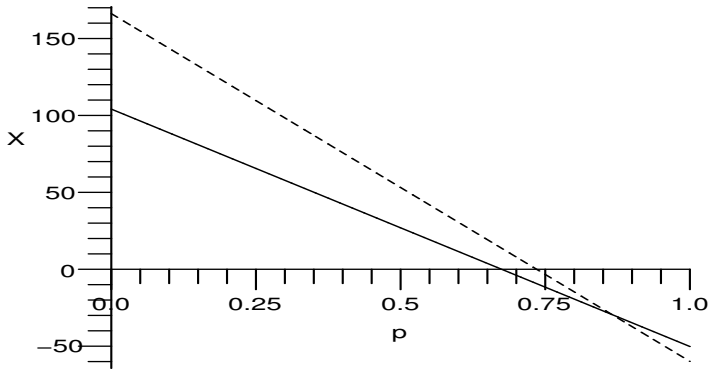

Figure 5.2: The plot of the parameter $X(\varrho_p)$ as a function of the amount of noise for noisy W-states of $N = 7$ qubits (solid line) and $N = 8$ qubits (dashed line).

5.6.1 Description of the experiment

Strings of up to eight $^{40}Ca^+$ ions are held in a linear ion trap capable of storing the ions for several days, a time sufficiently long for creating an entangled state more than 10^6 times. The qubits are encoded in superpositions of the $S_{1/2}$ ground state and the metastable $D_{5/2}$ state of the Ca^+ ions (lifetime of the $D_{5/2}$ level: $\tau \approx 1.16$ s). For the atomic level scheme, we refer to Fig. 5.3a. Each ion in the linear string is individually addressed by a series of tightly focused laser pulses on the $|1\rangle \equiv S_{1/2}(m_j = -1/2) \longleftrightarrow |0\rangle \equiv D_{5/2}(m_j = -1/2)$ quadrupole transition with narrowband laser radiation near 729 nm. Depending on its frequency, the laser couples either the states $|n\rangle_m|1\rangle \leftrightarrow |n\rangle_m|0\rangle$ (carrier pulse) or the states $|n\rangle_m|1\rangle \leftrightarrow |n+1\rangle_m|0\rangle$ (blue sideband pulse, laser detuned by $+\omega_z$ with respect to the atomic transition, see Fig. 5.3c). Here, $|n\rangle_m$ represent the vibrational states of the ion string's center–of–mass motion and n is the excitation number.

The N-ion W-states:

$$\begin{aligned} |0>_m |W_N\rangle &= \frac{1}{\sqrt{N}} \sum_i |\chi_i\rangle, \\ |\chi_i\rangle &= |0\rangle_m |x_N \ldots x_1\rangle, \\ x_k &= \begin{cases} 1, \text{ if } k = i \\ 0, \text{ if } k \neq i \end{cases} \end{aligned} \tag{5.79}$$

(note the reverse ordering of the qubits) are created by applying the sequence of laser pulses shown in Table 5.1 to the ions.

First, the $|0\rangle_m|111\cdots1\rangle$–state is prepared by N π–pulses on the carrier transition applied to ions #1 to #N. Then, laser light coupling the $|1\rangle$ state resonantly

Table 5.1: Creation of a $|W_N\rangle$–state ($N = \{6, 7, 8\}$). The numbers within the state vector refer to the phonon excitations of the center–of–mass mode of the ion crystal. The electronic states are labelled by $|1\rangle$ and $|0\rangle$. $R_n^c(\theta)$ denotes a carrier pulse of length θ applied to the ion n, $R_n^+(\theta)$ a blue sideband pulse. (i1) $\cdots$ (i3) mark initialization steps, (1) $\cdots$ (N) the actual entangling steps. Note that we count the atoms from right to left.

	$\|0\rangle_m\|111\cdots1\rangle$
(i1)	$\xrightarrow{R_N^C(\pi)R_{N-1}^C(\pi)\cdots R_1^C(\pi)}$
	$\|0\rangle_m\|000\cdots0\rangle$
	Check state via fluorescence
(i2)	$\xrightarrow{R_1^+(\pi)}$
	$\|0\rangle_m\|000\cdots0\rangle$
	Check state via fluorescence
(i3)	$\xrightarrow{R_N^C(\pi)}$
	$\frac{1}{\sqrt{N}}\|0\rangle_m\|100\cdots0\rangle$
(1)	$\xrightarrow{R_N^+(2\arccos(1/\sqrt{N}))}$
	$\frac{1}{\sqrt{N}}\|0\rangle_m\|100\cdots0\rangle + \frac{\sqrt{N-1}}{\sqrt{N}}\|1\rangle_m\|000\cdots0\rangle$
(2)	$\xrightarrow{R_{N-1}^+(2\arcsin(1/\sqrt{N-1}))}$
	$\frac{1}{\sqrt{N}}\|0\rangle_m\|100\cdots0\rangle + \frac{1}{\sqrt{N}}\|0\rangle_m\|010\cdots0\rangle + \frac{\sqrt{N-2}}{\sqrt{N}}\|1\rangle_m\|000\cdots0\rangle$
$\vdots$	$\vdots$
	$\frac{1}{\sqrt{N}}\|0\rangle_m\|100\cdots0\rangle + \frac{1}{\sqrt{N}}\|0\rangle_m\|010\cdots0\rangle + \cdots + \frac{1}{\sqrt{N}}\|1\rangle_m\|000\cdots0\rangle$
(N)	$\xrightarrow{R_1^+(2\arcsin(1/\sqrt{1}))}$
	$\frac{1}{\sqrt{N}}\|0\rangle_m\|100\cdots0\rangle + \frac{1}{\sqrt{N}}\|0\rangle_m\|010\cdots0\rangle + \cdots + \frac{1}{\sqrt{N}}\|0\rangle_m\|000\cdots1\rangle$

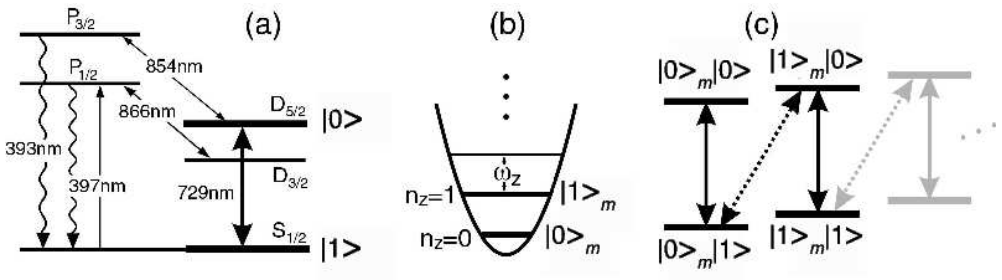

Figure 5.3: (a) Level scheme of Ca^+. (b) Schematics of the two lowest levels of the harmonic oscillator describing the bus mode. (c) Joint energy level diagram of the electronic qubit levels $\{|1\rangle,|0\rangle\}$ and the phonon numbers of the ion's motional mode used for entanglement generation $\{|0\rangle_m,|1\rangle_m\}$. Carrier transitions are marked as solid arrows, the blue sideband transition as a dashed arrow. Note that the $|0\rangle_m|0\rangle$–level does not couple to the blue sideband.

to the short-lived excited state $P_{1/2}$ projects the ion string on the measurement basis. Absence of fluorescence reveals whether all ions were prepared in $|0\rangle$. Similarly, we test the motional state with a single blue π pulse. Absence of fluorescence during a subsequent detection period indicates ground state occupation. This initialization procedure can be viewed as a generalized optical pumping with the target state $|0\rangle_m|11\cdots1\rangle$. If both checks were successful (total success rate ≥ 0.7), we continue with the $|W\rangle$–preparation at step $(i3)$ in Tab. 5.1 to create the state $|0\rangle_m|10\cdots0\rangle$. The entangling procedure starts by moving most of the population to the $|1\rangle_m|000\cdots0\rangle$ with a blue sideband pulse of pulse area $\theta_n = \arccos(1/\sqrt{n})$ leaving $1/N$ of the population back in $|0\rangle_m|100\cdots0\rangle$. Now, W–states are efficiently generated by redistributing the $|1\rangle_m|0\ldots0\rangle$ state population equally among the states $|0\rangle_m|0\ldots01_i0\ldots0\rangle, i = 1\ldots N-1$. This is achieved by $N-1$ blue sideband pulses of pulse length $\theta_n = \arcsin(1/\sqrt{n})$. Note that for an ion string in the motional ground state, blue–sideband pulses acting on an ion in the $|0\rangle$–state have no effect.

To verify the entanglement of the produced state, a measurement of a witness operator, yielding a negative expectation value, would be in principle sufficient. However, the optimal witness is a priori not known. Therefore, it can be advantageous to get as much information as possible about the produced quantum state. Full information on the N–ion entangled state is obtained through quantum state reconstruction, also called state tomography. For this, we expand the density matrix in a basis of observables, and measure (through ions' fluorescence) the corresponding expectation values. For the basis, we choose tensor products of Pauli matrices: $\sigma_N^{i_N}\otimes\ldots\otimes\sigma_1^{i_1}$ (note the reverse ordering). We use 3^N different bases and repeat the experiment 100 times for each basis. For $N = 8$, we need thus 656 100 experiments and a total measurement time of 10 hours. We follow the iterative procedure of Hradil *et al.* [42] for performing a maximum-likelihood estimation of the generated state ϱ_{ex}. The procedure ensures also positivity of the reconstructed matrix. The resulting matrix for the state $|W_7\rangle$ is displayed in Fig. 5.4, the numerical values are

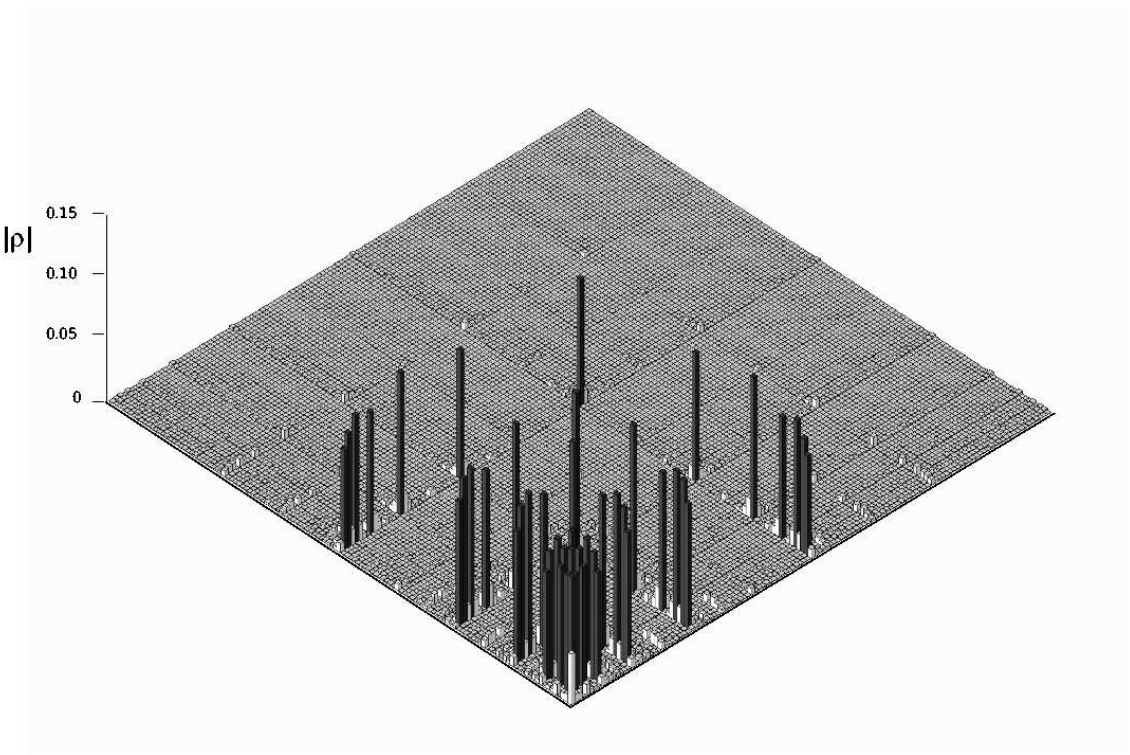

Figure 5.4: Absolute values of the reconstructed density matrix of a $|W_7\rangle$–state as obtained from quantum state tomography. Ideally, the dark entries should all have the same height of $\frac{1}{7}$, the bright bars should vanish.

available in the on-line material of Häffner *et al.* [36].

A Monte Carlo simulation is used to estimate uncertainties in the density matrix elements, and in quantities derived from it, that are due to quantum noise in the state reconstruction measurements: starting from the reconstructed density matrix, we simulate the measurement process and reconstruct up to 100 times the density matrix from these simulated measurements. From the set of reconstructed density matrices, the spread in the expectation values of the observable of interest can be estimated. For density matrices close to pure states, we observe that the purity of the reconstructed matrices often slightly decreases (for the W-states by about 2%). Therefore, we conclude that the reconstruction process rather underestimates the entanglement in the experimentally produced quantum states.

5.6.2 Evaluation of the data

In the work of Häffner *et al.* [36] it has already been shown that the states are genuine multipartite entangled, multipartite distillable, and also that all the reduced two-qubit states are entangled. Now we want to apply our criteria to the experimental density matrices ϱ_{ex}.

We begin with the 7-qubit states. In this case, the fidelity $F_N := \langle W_N|\varrho_{ex}\, W_N\rangle$ of the produced states was $F_7 = 0.763$. To check the presence of bipartite entanglement, we use the inequality (5.24) rather than (5.26), as the experimental states are not symmetric due to the experimental imperfections described in the previous Subsection. According to the theoretical analysis of Section 5.5 (c.f. formula (5.50)), the frame directions $\mathbf{k}, \mathbf{l}, \mathbf{n} = x, y, z$. We find that:

$$\langle (J^z)^2\rangle + \frac{N(N-2)}{4} = 14.666 \pm 0.016\,,$$

$$\sqrt{\Big[\langle (J^x)^2\rangle + \langle (J^y)^2\rangle - \frac{N}{2}\Big]^2 + (N-1)^2\langle J^z\rangle^2} = 15.148 \pm 0.023\,,$$

which clearly proves the presence of bipartite entanglement in the produced states.

Let us move to the tripartite entanglement. We evaluate $X(\varrho_{ex})$ using the Lorenz matrix (5.75). We find that:

$$X(\varrho_{ex}) = -24.937 \pm 0.202\,, \tag{5.80}$$

and hence the spin squeezing inequality (5.37) is fulfilled. However, as we mentioned at the end of Section 5.3, the validity of the inequality (5.37) only proves the presence of *some* form of tripartite entanglement and a priori we do not know if it is genuine 3-qubit entanglement.

Let us now discuss the eight qubit case. Here, the experimentally reached fidelity was $F_8 = 0.7215$. The evaluation of the bipartite criteria yields:

$$\langle (J^z)^2\rangle + \frac{N(N-2)}{4} = 20.462 \pm 0.007\,,$$

$$\sqrt{\Big[\langle (J^x)^2\rangle + \langle (J^y)^2\rangle - \frac{N}{2}\Big]^2 + (N-1)^2\langle J^z\rangle^2} = 20.838 \pm 0.009\,,$$

and the tripartite criterion gives:

$$X(\varrho_{ex}) = -29.017 \pm 0.2623. \tag{5.81}$$

Thus, both criteria detect entanglement again.

5.7 Simplified criteria for genuine 3-qubit entanglement

The search for the Lorenz matrices Λ, L in Theorem 5.2 can be difficult due to non-compactness of the restricted Lorenz group. It is therefore desirable to develop some simpler conditions as well. For mesoscopic systems with not too large N we may do so, using some specific witnesses that detect genuine GHZ-type, or genuine W-type entanglement (c.f. Section 5.1.1), found by Acín *et al.* in Ref. [2]:

$$\mathcal{W}_{GHZ} := \frac{3}{4}\mathbf{1} - |GHZ_3\rangle\langle GHZ_3|, \tag{5.82}$$

$$\mathcal{W}_{W_1} := \frac{2}{3}\mathbf{1} - |W_3\rangle\langle W_3|, \tag{5.83}$$

$$\mathcal{W}_{W_2} := \frac{1}{2}\mathbf{1} - |GHZ_3\rangle\langle GHZ_3|\,, \tag{5.84}$$

where now we allow the vectors $|GHZ_3\rangle$ and $|W_3\rangle$ to be defined in an arbitrary frame $\mathbf{k}, \mathbf{l}, \mathbf{n}$, the same for all three qubits. Apart from the simplicity, the advantage of such an approach over the general criterion (5.37) is that the above witnesses detect genuine 3 qubit entanglement in generic states: the witnesses $\mathcal{W}_{GHZ}$ detects states of GHZ-class which are neither of the W-class, nor biseparable; the witnesses $\mathcal{W}_{W_1}$ and $\mathcal{W}_{W_2}$ detect states of GHZ- or W-class, which are not biseparable.

We derive the spin squeezing inequalities corresponding to $\mathcal{W}_{GHZ}$, $\mathcal{W}_{W_1}$, $\mathcal{W}_{W_2}$ using the same technique as in Section 5.3: we express the sums

$$\sum_{\langle abc\rangle} \mathrm{tr}_{abc}\big(\varrho_{abc}\mathcal{W}_{abc}\big) = \mathrm{tr}\big(\varrho \sum_{\langle abc\rangle} \mathcal{W}_{abc}\big) \tag{5.85}$$

with the total spin operators (5.3). However, instead of using the general formula (5.35), we can calculate explicitly the occurring products of Pauli matrices (or in other words we use special cases of Eq. (5.35)). This leads us to the following criteria:

Proposition 5.2 (GHZ-type entanglement). *If for a state ϱ there exist orthogonal directions $\mathbf{k}, \mathbf{l}, \mathbf{n}$ such that the following inequality is fulfilled:*

$$-\frac{1}{3}\langle J^3_{\mathbf{k}}\rangle + \langle J_{\mathbf{l}} J_{\mathbf{k}} J_{\mathbf{l}}\rangle - \frac{N-2}{2}\langle J^2_{\mathbf{n}}\rangle + \frac{1}{3}\langle J_{\mathbf{k}}\rangle + \frac{N(N-2)(5N-2)}{24} < 0\,, \tag{5.86}$$

then the state ϱ possesses a genuine GHZ-type entanglement.

Proposition 5.3 (GHZ- or W-type entanglement). *If for a state ϱ there exist orthogonal directions $\mathbf{k}, \mathbf{l}, \mathbf{n}$ such that one of the following inequalities is fulfilled:*

$$\begin{aligned}\langle J^3_{\mathbf{n}}\rangle - 2\langle J_{\mathbf{l}} J_{\mathbf{n}} J_{\mathbf{l}}\rangle - 2\langle J_{\mathbf{k}} J_{\mathbf{n}} J_{\mathbf{k}}\rangle - \frac{N-2}{2}\Big(2\langle J^2_{\mathbf{k}}\rangle + 2\langle J^2_{\mathbf{l}}\rangle - \langle J^2_{\mathbf{n}}\rangle\Big) \\ - \frac{N^2-4N+8}{4}\langle J_{\mathbf{n}}\rangle + \frac{N(N-2)(13N-4)}{24} < 0,\end{aligned} \tag{5.87}$$

$$-\frac{1}{3}\langle J^3_{\mathbf{k}}\rangle + \langle J_{\mathbf{l}} J_{\mathbf{k}} J_{\mathbf{l}}\rangle - \frac{N-2}{2}\langle J^2_{\mathbf{n}}\rangle + \frac{1}{3}\langle J_{\mathbf{k}}\rangle + \frac{N^2(N-2)}{8} < 0\,, \tag{5.88}$$

then the state ϱ possesses a genuine 3-qubit (GHZ- or W-type) entanglement.

The witnesses (5.82)-(5.84) still have a disadvantage that in the sums $\sum_{\langle abc\rangle}\mathcal{W}_{abc}$, the identity gives the dominant contribution and hence the bigger the system the less sensitive the witnesses become. One possible method to partially overcome this problem is to project the witnesses (5.82-5.84) onto the symmetric subspace of the space of three qubits:

$$\widetilde{\mathcal{W}}_{GHZ} := \frac{3}{4}P_3 - |GHZ_3\rangle\langle GHZ_3|, \tag{5.89}$$

$$\widetilde{\mathcal{W}}_{W_1} := \frac{4}{9}P_3 - |W_3\rangle\langle W_3|, \tag{5.90}$$

$$\widetilde{\mathcal{W}}_{W_2} := \frac{1}{2}P_3 - |GHZ_3\rangle\langle GHZ_3|\,, \tag{5.91}$$

where:

$$P_3 := |000\rangle\langle 000| + |111\rangle\langle 111| + |W_3\rangle\langle W_3| + |W_3'\rangle\langle W_3'|. \tag{5.92}$$

The factor 4/9 in the definition (5.90) is the maximum overlap between $|W_3\rangle$ and symmetric separable states (recall that there are no symmetric biseparable states due to the symmetry). The criteria that such improved witnesses lead to, i.e. the analogs of inequalities (5.86 -5.88), read respectively:

$$-\frac{1}{3}\langle J_{\mathbf{k}}^3\rangle + \langle J_{\mathbf{l}}J_{\mathbf{k}}J_{\mathbf{l}}\rangle + \frac{N-2}{2}\langle J_{\mathbf{k}}^2 + J_{\mathbf{l}}^2\rangle + \frac{1}{3}\langle J_{\mathbf{k}}\rangle + \frac{N(N-2)(N-4)}{12} < 0, \tag{5.93}$$

for the GHZ-type entanglement, and

$$\langle J_{\mathbf{n}}^3\rangle - 2\langle J_{\mathbf{l}}J_{\mathbf{n}}J_{\mathbf{l}}\rangle - 2\langle J_{\mathbf{k}}J_{\mathbf{n}}J_{\mathbf{k}}\rangle + \frac{N-2}{9}\left(\frac{25}{2}\langle J_{\mathbf{n}}^2\rangle - \langle J_{\mathbf{l}}^2 + J_{\mathbf{k}}^2\rangle\right) - \frac{N^2-4N+8}{4}\langle J_{\mathbf{n}}\rangle + \frac{7N(N-2)(N-4)}{72} < 0, \tag{5.94}$$

$$-\frac{1}{3}\langle J_{\mathbf{k}}^3\rangle + \langle J_{\mathbf{l}}J_{\mathbf{k}}J_{\mathbf{l}}\rangle + \frac{N-2}{12}\Big(2\langle J_{\mathbf{k}}^2 + J_{\mathbf{l}}^2\rangle - \langle J_{\mathbf{n}}^2\rangle\Big) + \frac{1}{3}\langle J_{\mathbf{k}}\rangle + \frac{N(N-2)(N-4)}{48} < 0\,. \tag{5.95}$$

for the GHZ- or W-type entanglement.

The potential advantage of using $\widetilde{\mathcal{W}}_{GHZ}$, $\widetilde{\mathcal{W}}_{W_1}$, and $\widetilde{\mathcal{W}}_{W_2}$ instead of $\mathcal{W}_{GHZ}$, $\mathcal{W}_{W_1}$, and $\mathcal{W}_{W_2}$ manifests itself only for non-symmetric states. For symmetric states, both families give the same results (apart from $\widetilde{\mathcal{W}}_{W_1}$ due to the factor 4/9), as we can always substitute ϱ_{abc} with $P_3\,\varrho_{abc}\,P_3$ in Eq. (5.85).

Finally, let us apply the above witnesses to the Dicke states $|\Psi_{N,k}\rangle$ of Section 5.5. As one can easily see from Eq. (5.54), only $\mathcal{W}_{W_1}$ and $\widetilde{\mathcal{W}}_{W_1}$ have a chance to detect genuine tripartite entanglement, however not for all N and k. For example, for $|W_N\rangle$, $\mathcal{W}_{W_1}$ detects entanglement only for $N \leq 4$, and $\widetilde{\mathcal{W}}_{W_1}$ — only for $N \leq 6$.

5.8 Concluding remarks

The novel inequalities, which we developed in this Chapter, similarly as the squeezing parameter ξ^2, i) have a clear physical meaning in terms of generalized squeezing and entanglement conditions, ii) can be relatively easy measured, and iii) are given by complex, but *elementary* expressions.

Although we studied only 2- and 3-qubit entanglement here, the generalization of the proposed method to study the entanglement between more qubits is straightforward — one uses inequalities of the type $\mathrm{tr}\big(\varrho\mathcal{W}\big) < 0$ with appropriable witnesses $\mathcal{W}$. However, for the case of four or more qubits the PPT criterion is no longer a necessary separability condition and only sufficient entanglement conditions of the type (5.86)-(5.88) and (5.93)-(5.95) can be obtained.

Chapter 6

Statistical-mechanical description of quantum entanglement

In this Chapter we present a novel description of finite dimensional quantum entanglement, based on a study of the space of all convex decompositions of a given density matrix. On this space we construct a system of real polynomial equations describing separable states. We further study this system using statistical mechanical methods. Finally, we apply our techniques to Werner states of two qubits and obtain a sufficient criterion for separability.

6.1 Separability test on the space of ϱ-ensembles

In Section 3.1.2 we mentioned that the difficulty of the separability problem lies in the fact that a convex decomposition of a given mixed state ϱ into pure states:

$$\varrho = \sum_{i=1}^{N} p_i \, |\psi_i\rangle\langle\psi_i| \tag{6.1}$$

is highly non-unique. Thus, the following Definition makes sense:

Definition 6.1. *An unordered collection $\{p_i, |\psi_i\rangle\}$, $i = 1 \dots N$ of probabilities and vectors satisfying (6.1) is called a ϱ-ensemble of length N.*

In this Chapter we develop the following approach to the separability problem: we propose to search the space of all ϱ-ensembles of a given state ϱ for product ϱ-ensembles (ϱ-ensembles containing only product vectors), by applying one of the existing necessary and sufficient entanglement tests to each member of the ensemble. Among the available test, we choose the one given by Proposition 3.1 from Section 3.1.2 due to its simplicity — in order to check a vector $|\psi\rangle$, it is enough to calculate

a fourth-order polynomial function of $|\psi\rangle$. This leads to a set of real polynomial equations describing separable states. The resulting system is somewhat simpler than the one given by Eq. (3.5), but still very complicated due to the fourth order of some equations and a large number of variables. Our idea is to study it using methods of classical statistical mechanics. The motivation is that such methods have proven to be very efficient not only within classical mechanics, but also in many other, distantly related areas (for an application to fundamental combinatorial problems see e.g. Kubasiak *et al.* [57] and the references therein). Hence, we first develop a mechanical analogy for our system. Then we define a suitable "energy", introduce a canonical ensemble, and study the resulting partition function.

Let us begin with describing the space of all ϱ-ensembles of a given state ϱ. Just like in Chapter 3, we consider here a composite system described by a finite dimensional Hilbert space $\mathcal{H} = \mathbb{C}^m \otimes \mathbb{C}^n$. For technical reasons it will be easier to pass from normalized ϱ-ensemble vectors $|\psi_i\rangle$ to subnormalized ones: $\sqrt{p_i}|\psi_i\rangle$, which we denote by the same letter, so that: $\varrho = \sum_{i=1}^{N} |\psi_i\rangle\langle\psi_i|$. Let us fix an eigenensemble $\{|e_\alpha\rangle\}$ of ϱ, where all the vectors $|e_\alpha\rangle$ correspond to nonzero eigenvalues λ_α of ϱ, $\alpha = 1 \ldots r$, and $r := \mathrm{rk}(\varrho)$ is the rank of ϱ. Then the following fact holds (Hughston *et al.* [43]):

Theorem 6.1 (Schrödinger-Hughston-Jozsa-Wootters). *Any ϱ-ensemble $\{|\psi_i\rangle\}$ of length $N \geq r$ can be obtained from the eigenensemble $\{|e_\alpha\rangle\}$ through the following linear transformation:*

$$|\psi_i\rangle := \sum_{\alpha=1}^{r} z_{i\alpha}|e_\alpha\rangle, \tag{6.2}$$

where matrix $z_{i\alpha} \in \mathbb{C}$ satisfies:

$$\sum_{i=1}^{N} \overline{z_{i\alpha}} z_{i\beta} = \delta_{\alpha\beta}. \tag{6.3}$$

Proof. From Eqs. (6.2) and (6.3) we easily obtain that:

$$\sum_i |\psi_i\rangle\langle\psi_i| = \sum_{\alpha,\beta} \sum_i \overline{z_{i\alpha}} z_{i\beta} |e_\beta\rangle\langle e_\alpha| = \sum_\alpha |e_\alpha\rangle\langle e_\alpha| = \varrho, \tag{6.4}$$

so that the vectors defined by Eq. (6.2) indeed form a ϱ-ensemble.

On the other hand, for any ϱ-ensemble $\{|\psi_i\rangle\}$ define $z_{i\alpha} := \langle e_\alpha|\psi_i\rangle/\lambda_\alpha$. Such defined $z_{i\alpha}$ satisfies Eq. (6.3), as we have assumed that the eigenvectors $|e_\alpha\rangle$ are subnormalized: $\langle e_\alpha|e_\beta\rangle = \lambda_\alpha \delta_{\alpha\beta}$. Moreover, for some i let $|\psi_i\rangle$ possess a non-zero component $|\psi_\perp\rangle$, orthogonal to $\mathrm{Ran}(\varrho) := \mathrm{span}_{\mathbb{C}}\{e_1, \ldots, e_r\}$, so that $|\psi_i\rangle = \sum_\alpha z_{i\alpha}|e_\alpha\rangle + |\psi_\perp\rangle$. But then one would have that $\varrho|\psi_\perp\rangle \neq 0$, which is impossible, since the decomposition $\mathcal{H} = \mathrm{Ker}(\varrho) \oplus \mathrm{Ran}(\varrho)$ implies that $|\psi_\perp\rangle \in \mathrm{Ker}(\varrho)$. □

Thus, Theorem 6.1 gives us the characterization of all possible ϱ-ensembles in terms of $N \times r$ matrices z, satisfying the condition (6.3). Geometrically, this condition defines the, so called, compact Stiefel manifold $V_{N,r} := U(N)/U(N-r)$ (we

refer to Spivak vol. 5 [92] for more details on the Stiefel manifolds). However, note that there is some additional symmetry: from Eq. (6.1) we see that the order of vectors in a ϱ-ensemble does not matter, and thus two $N \times r$ matrices z, z' satisfying Eq. (6.3) and differing only by permutation of their rows define the same ϱ-ensemble. To fix this freedom, observe that a matrix satisfying Eq. (6.3) has necessarily rank r, and hence we may consider only those matrices z, for which the first r rows are linearly independent. Thus, out of the whole $V_{N,r}$ it is enough to consider only one open coordinate neighbourhood. But then the Eq. (6.3) can be solved, yielding:

$$z = GS \begin{pmatrix} \mathbf{1}_r \\ \mathbf{v} \end{pmatrix} \cdot u, \quad , \tag{6.5}$$

where $u \in U(r)$, $\mathbf{1}_r$ is the $r \times r$ unit matrix, $\mathbf{v}$ is an arbitrary complex $(N-r) \times r$ matrix, and GS denotes the Gram-Schmidt orthonormalization[1] applied to the columns. There are no more symmetries, since we have defined in Definition 6.1 ϱ-ensembles using vectors $|\psi_i\rangle$ rather than more physical projectors $|\psi_i\rangle\langle\psi_i|$, as the latter are harder to work with. In case of ϱ-ensembles defined through projectors, there would be an additional symmetry of multiplying each row of z by a (different) phase.

So far we have characterized ϱ-ensembles of a fixed length N. It seems that in the search for product ensemble we would have to consider all lengths $N \geq r$. However, from Caratheodory's Theorem (Section 3.1.2) we know that a separable state can be decomposed into at most $N = m^2n^2$ affinely independent (in $\mathbb{R}^{m^2n^2-1}$) product states. Hence, it is enough to consider only ϱ-ensembles of the length $N = m^2n^2$ (there is a natural inclusion of space of shorter ensembles in the space of longer ones).

Let us now examine the entanglement test given by Proposition 3.1 from Section 3.1.2: $|\psi\rangle$ is product if and only if

$$||\psi||^4 - \mathrm{tr}_1\big(\mathrm{tr}_2|\psi\rangle\langle\psi|\big)^2 = 0. \tag{6.6}$$

Since left hand side of Eq. (6.6) is non-negative for any $|\psi\rangle$, we can sum up the conditions (6.6) for all ensemble members of a given ϱ-ensemble and thus obtain the test for the whole ϱ-ensemble. Combining this with the parametrizations (6.2), (6.3), we obtain the following description of separable states:

Proposition 6.1. *A states ϱ of rank r is separable if and only if the following system*

[1]The Gram-Schmidt orthogonalization creates an orthonormal basis of a span of a set $\{|v_1\rangle, \ldots, |v_r\rangle\}$ of a linearly independent vectors form some Hilbert space. Define:

$$|\widetilde{u}_1\rangle := |v_1\rangle, \quad |\widetilde{u}_i\rangle := |v_i\rangle - \sum_{j=1}^{r-1} \frac{\langle \widetilde{u}_j|v_i\rangle}{||\widetilde{u}_j||^2} |\widetilde{u}_j\rangle.$$

Then $\{\widetilde{u}_1, \ldots, \widetilde{u}_r\}$ is a orthogonal system and spans the same space as $\{v_1, \ldots, v_r\}$. Passing to the normalized vectors: $|u_i\rangle := \frac{1}{||\widetilde{u}_i||^2} |\widetilde{u}_i\rangle$, we obtain the desired orthonormal system.

of real polynomial equations possesses a solution:

$$F_\varrho(z) := \sum_{i=1}^{m^2n^2} \sum_{\alpha,\ldots,\nu=1}^{r} \overline{z_{i\alpha}}\,\overline{z_{i\beta}} F_{\alpha\beta\mu\nu} z_{i\mu} z_{i\nu} = 0, \tag{6.7}$$

$$c_{\alpha\beta}(z) := \sum_{i=1}^{m^2n^2} \overline{z_{i\alpha}} z_{i\beta} - \delta_{\alpha\beta} = 0, \tag{6.8}$$

where:

$$F_{\alpha\beta\mu\nu} := \langle e_\alpha \otimes e_\beta | \Pi_m \otimes \Pi_n \, e_\mu \otimes e_\nu \rangle \tag{6.9}$$

and Π_m, Π_n *denote the projectors onto the skew-symmetric spaces* $\mathbb{C}^m \wedge \mathbb{C}^m$ *and* $\mathbb{C}^n \wedge \mathbb{C}^n$ *respectively.*

The left hand side of Eq. (6.7) is closely related to the generalized concurrence for pure states (Rungta *et al.* [84]), however the latter is not a polynomial function of the tested vector.

A similar analysis leading to a set of polynomial equations was also carried out by Wu *et al.* in Ref. [111]. However, these authors used another, higher order polynomial test for entanglement. Let $\sigma_1 := \mathrm{tr}_2 |\psi\rangle\langle\psi|$, then $|\psi\rangle$ is product if and only if $\det(\sigma_1 - \mathbf{1}) = 0$. The relation to Eq. (6.6) is established by observing that $\det(\sigma_1 - \mathbf{1}) = \sum_{k=0}^{m} (-1)^k c_k(\sigma_1)$, where c_k's form a basis of $U(m)$-invariant polynomials (see e.g. Kobayashi and Nomizu vol. 2 [48]). Particularly, $2c_2(\sigma_1) = \big(\mathrm{tr}\sigma_1\big)^2 - \mathrm{tr}\sigma_1^2$, which is just the left hand side of Eq. (6.6). Hence, for testing entanglement, out of all polynomials c_k it is enough to apply only c_2.

6.2 Statistical-mechanical description

The polynomial system (6.7), (6.8), just like any system of real polynomials, can be in principle analyzed using the Real Nullstellensatz and the certificate (3.6), we mentioned in Section 3.1.2. However, finding such certificate is very computationally demanding.

Here we develop another approach, based on a particular classical mechanical analogy. Namely, we can look at $z_{i\alpha}$ as at a collection of complex row vectors $\mathbf{z}_i \in \mathbb{C}^r$, $i = 1 \ldots N$ and treat each row $\mathbf{z}_i$ as a complex phase-space coordinate of a fictitious particle in r-dimensional space. Then the whole $z_{i\alpha}$ is a phase-space coordinate of a system of N such particles. Now, let $F_\varrho(\mathbf{z}_1, \ldots, \mathbf{z}_N)$ and $c_{\alpha\beta}(\mathbf{z}_1, \ldots, \mathbf{z}_N)$ be defined by Eqs. (6.7) and (6.8). We emphasize that F depends on the analyzed state ϱ through the fixed eigenensemble $\{|e_\alpha\rangle\}$. Since the entanglement function F_ϱ is real, non-negative, and extensive, we may think of it as of the Hamiltonian of our fictitious mechanical system. Then, we can look at $c_{\alpha\beta}$ as at the primary constraints, imposed on the a priori independent variables $z_{i\alpha}$. Note that the interparticle interaction is encoded in the constraints and not in the Hamiltonian F_ϱ. Although we can solve the constraints explicitly by Eq. (6.5), the resulting parametrization of

the constrained manifold is rather hard to work with due to the iterative nature of the Gram-Schmidt orthonormalization. Thus, we choose to proceed using the standard method of treatment of constrained systems due to Dirac [16]. This method is very powerful and universal (see e.g. our work [49] on a null-surface Hamiltonian formalism in general relativity). We define the full Hamiltonian of the systems as:

$$H_{full}(\mathbf{z}_1 \dots \mathbf{z}_N) := F_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) + \sum_{\alpha,\beta} \omega_{\alpha\beta} c_{\alpha\beta}(\mathbf{z}_1 \dots \mathbf{z}_N) \ , \tag{6.10}$$

where $\omega_{\alpha\beta}$ are Lagrange multipliers. Note that since the matrix defined by $c_{\alpha\beta}$ is hermitean, we take ω hermitean too, so that H_{full} is real. Moreover, in order to take into account all independent constraints, we require that $\det \omega \neq 0$. Then the constraints $c_{\alpha\beta} = 0$ are restored by setting to zero the variation of H_{full} with respect to $\omega_{\alpha\beta}$: $\partial H_{full}/\partial \omega_{\alpha\beta} = 0$. The system (6.7), (6.8) thus describes a global minimum of the constrained Hamiltonian (6.10) (recall that $F_\varrho \geq 0$).

The number of fictitious particles N is rather large — for example in dimension $3 \otimes 3$ we have $N = 81$. Thus, the direct study of our fictitious mechanical system seems rather hopeless and we proceed further using methods of statistical mechanics. The most natural framework would be microcanonical ensemble, however it is also difficult to work with. Hence, we will introduce a canonical ensemble, keeping in mind that this is just a technical tool, so for example the inverse temperature β plays only a role of a parameter here, without any physical meaning. Ultimately, we are interested in the low temperature limit $\beta \to \infty$.

In order to define the partition function Z for the Hamiltonian (6.10), we first rescale the variables: $z_{i\alpha} \mapsto z_{i\alpha}/\sqrt{N}$ and then set[2] :

$$Z(\beta, \omega; \varrho) := \int \prod_{i,\mu} \mathrm{d}^2 z_{i\mu} \exp\Big[- \frac{\beta}{N^2} \Big(F_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) + N \sum_i \langle \mathbf{z}_i | \omega \mathbf{z}_i \rangle - N^2 \mathrm{tr}\omega \Big) \Big], \tag{6.12}$$

where $\langle \cdot \,|\, \cdot \rangle$ denotes the standard scalar product in $\mathbb{C}^r$. Performing further rescaling:

$$\beta = N^2 \beta' \,, \quad \omega = \frac{N}{\beta} \omega' \,, \tag{6.13}$$

Z becomes (after dropping the primes):

$$Z(\beta, \omega; \varrho) = \int \prod_{i,\mu} \mathrm{d}^2 z_{i\mu} \exp\Big[- \beta F_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) - \sum_i \langle \mathbf{z}_i | \omega \mathbf{z}_i \rangle + N \mathrm{tr}\omega \Big] . \tag{6.14}$$

Note that now we are able to reproduce the (rescaled) constraints (6.8) only on average:

$$\frac{\partial}{\partial \omega_{\alpha\beta}} \log Z(\beta, \omega; \varrho) = 0 \ \Leftrightarrow \ \langle \langle \sum_i \overline{z_{i\alpha}} z_{i\beta} - N \delta_{\alpha\beta} \rangle \rangle = 0, \tag{6.15}$$

[2]The other possibility would be to explicitly restrict the integration in Eq. (6.16) to the constraint surface

$$Z(\beta; \varrho) = \int \prod_{i,\mu} \mathrm{d}^2 z_{i\mu} \delta(\phi(\mathbf{z}_1 \dots \mathbf{z}_N)) \, \mathrm{e}^{-\beta F_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N)}. \tag{6.11}$$

However this approach is less feasible. Alternatively what follows can be understood as an evaluation of the integral (6.11) by the stationary phase method.

where the average $\langle\langle \cdot \rangle\rangle$ is taken with respect to the probability density defined through Eq. (6.14). Following the standard treatment of constrained systems, the equations (6.15) are treated as conditions imposed on a priori arbitrary (apart form being hermitean and non-singular) matrix ω.

A significant simplification of the partition function (6.14) follows from the form of our Hamiltonian F_ϱ — from Eq. (6.7) it follows that $F_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) = \sum_i F_{1\,\varrho}(\mathbf{z}_i)$, where $F_{1\,\varrho}$ is just the function F_ϱ with $N = 1$. This leads to the factorization of the partition function: $Z(\beta, \omega; \varrho) = [Z_1(\beta, \omega; \varrho)]^N$, where Z_1 is the one-particle partition function:

$$Z_1(\beta, \omega; \varrho) := \int \prod_{\mu=1}^{r} \mathrm{d}^2 z_\mu \exp\Big[- \beta F_{1\,\varrho}(\mathbf{z}) - \langle \mathbf{z} | \omega \mathbf{z} \rangle + \mathrm{tr}\omega \Big]. \tag{6.16}$$

From now on we will consider Z_1 only. The constraint equations (6.15) are then replaced by the one-particle version:

$$\frac{\partial}{\partial \omega_{\alpha\beta}} \log Z_1(\beta, \omega; \varrho) = 0 \Leftrightarrow \ \langle\langle \overline{z_\alpha} z_\beta - \delta_{\alpha\beta} \rangle\rangle = 0 \ , \tag{6.17}$$

where the average is taken with respect to the probability distribution:

$$P_\varrho(\mathbf{z}; \beta, \omega) := \frac{1}{Z_1(\beta, \omega; \varrho)} \exp\Big[- \beta F_{1\,\varrho}(\mathbf{z}) - \langle \mathbf{z} | \omega \mathbf{z} \rangle + \mathrm{tr}\omega \Big]. \tag{6.18}$$

To understand the meaning of Eq. (6.17), let us assume that $\omega = \omega_0(\beta)$ is such that Eq. (6.17) is satisfied. Then Eq. (6.17) implies that a family of vectors $\{\psi(\mathbf{z}) := \sum_\alpha z_\alpha e_\alpha \, ; \, \mathbf{z} \in \mathbb{C}^r\}$ forms a continuous ϱ-ensemble with respect to the probability distribution (4.34), i.e.:

$$\int \mathrm{d}^r \mathbf{z} P_\varrho(\mathbf{z}; \beta, \omega_0) \, |\psi(\mathbf{z})\rangle\langle\psi(\mathbf{z})| = \varrho \tag{6.19}$$

irrespectively of β. The average entanglement of this ensemble is given by the average "energy" of the system, i.e. the average of the one-particle Hamiltonian $F_{1\,\varrho}$:

$$\langle\langle F_{1\,\varrho} \rangle\rangle_0(\beta) := \int \mathrm{d}^r \mathbf{z} \, P_\varrho(\mathbf{z}; \beta, \omega_0(\beta)) \, F_{1\,\varrho}(\mathbf{z}) = - \frac{\partial}{\partial \beta} \log Z_1 \Big|_{\omega = \omega_0(\beta)}. \tag{6.20}$$

Now, if in the limit of low temperature $\beta \to \infty$ one has that $\langle\langle F_{1\,\varrho} \rangle\rangle_0 \to 0$, then the given state ϱ possesses a continuous ensemble which is "on average" separable. The relation of such defined separability "on average" to actual separability is not clear yet. The intuition behind our statistical mechanical approach is that for a separable state ϱ which possesses sufficiently many separable ϱ-ensembles, i.e. $F_\varrho = 0$ on a set of non-zero measure on $V_{N,r}$, the partition function (6.16) should behave differently than for states with many entangled ensembles. In the next Section we will examine the behaviour of Z_1 for a simple example of the, so called, Werner states.

6.3 Calculation for Werner states

In this Section we apply the developed statistical method to study the Werner states of a $2 \otimes 2$ dimensional system. They were introduced by Werner in Ref. [102] and can be defined as follows:

$$w(p) := (1-p)|\Psi_-\rangle\langle\Psi_-| + \frac{p}{4}\mathbf{1}_2 \otimes \mathbf{1}_2, \tag{6.21}$$

where:

$$|\Psi_\pm\rangle := \frac{1}{\sqrt{2}}\big(|01\rangle \pm |10\rangle\big), \quad |\Phi_\pm\rangle := \frac{1}{\sqrt{2}}\big(|00\rangle \pm |11\rangle\big) \tag{6.22}$$

are the, so called, Bell basis states and $\{|0\rangle, |1\rangle\}$ is the standard basis of $\mathbb{C}^2$. The states $w(p)$ have positive partial transpose and hence are separable for $p \geq 2/3$.

As the fixed eigenensemble $\{|e_\alpha\rangle\}$ of $w(p)$ we take:

$$|e_1\rangle := \sqrt{1 - \frac{3}{4}p}\,|\Psi_-\rangle, \quad |e_2\rangle := \frac{\sqrt{p}}{2}\,\mathrm{i}|\Psi_+\rangle, \tag{6.23}$$

$$|e_3\rangle := \frac{\sqrt{p}}{2}\,\mathrm{i}|\Phi_-\rangle, \qquad |e_4\rangle := \frac{\sqrt{p}}{2}|\Phi_+\rangle. \tag{6.24}$$

In what follows we assume $p > 0$. Calculation of $F_{\alpha\beta\mu\nu}$ from Eq. (6.9) yields:

$$F_1(\mathbf{z}; p) = \frac{1}{64}\big|(4-3p)z_1^2 + pz_2^2 + pz_3^2 + pz_4^2\big|^2 \tag{6.25}$$

and hence:

$$Z_1(\beta, \omega; p) = \int \mathrm{d}^2 z_1 \ldots \mathrm{d}^2 z_4 \exp\Big[-\beta\,\big|(4-3p)z_1^2 + pz_2^2 + pz_3^2 + pz_4^2\big|^2 - \langle \mathbf{z}|\omega\mathbf{z}\rangle + \mathrm{tr}\omega\Big] \tag{6.26}$$

(we have absorbed the factor $1/64$ into the definition of the parameter β). Since the fourth-order term in the exponent is a squared modulus of a second order polynomial, we can perform the Hubbard-Stratonovitch trick and substitute:

$$\exp(-\beta|y|^2) = \int \frac{\mathrm{d}^2 s}{\pi\beta} \exp\left(-\frac{|s|^2}{\beta} + \mathrm{i}\,\overline{s}y + \mathrm{i}s\overline{y}\right). \tag{6.27}$$

This gives:

$$\begin{aligned} Z_1(\beta, \omega; p) = &\int \frac{\mathrm{d}^2 s}{\pi\beta} \int \frac{1}{2^4} \mathrm{d}z_1 \ldots \mathrm{d}z_4\, \mathrm{d}\overline{z}_1 \ldots \mathrm{d}\overline{z}_4 \\ &\times \exp\Big\{ \mathrm{i}\overline{s}\Big[(4-3p)z_1^2 + pz_2^2 + pz_3^2 + pz_4^2\Big] + \mathrm{i}s\Big[(4-3p)\overline{z}_1^{\,2} + p\overline{z}_2^{\,2} \\ &+ p\overline{z}_3^{\,2} + p\overline{z}_4^{\,2}\Big] - \langle \mathbf{z}|\omega\mathbf{z}\rangle + \mathrm{tr}\omega \Big\}. \end{aligned} \tag{6.28}$$

The sufficient condition for the above integral to exist is that $\omega > 0$ (as we said earlier we take ω non-singular, hence the strong inequality here). This puts no restriction on the amount of independent parameters in ω and from now on we will

assume this condition to hold. Performing the Gaussian integration in Eq. (6.28) we obtain:

$$Z_1(\beta,\omega;p)=\frac{\pi^3}{\beta}\int \mathrm{d}^2 s\,\mathrm{e}^{-|s|^2/\beta+\mathrm{tr}\omega}\frac{1}{\sqrt{\det M}}, \tag{6.29}$$

where M is a 8×8 matrix defined as follows:

$$M:=\begin{bmatrix} \omega & -2\mathrm{i}sI(p) \\ -2\mathrm{i}\,\overline{s}\,I(p) & \overline{\omega} \end{bmatrix}, \quad I(p):=\begin{bmatrix} 4-3p & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{bmatrix}. \tag{6.30}$$

To calculate $\det M$ for $p\neq 0$ we first perform a transformation:

$$M\mapsto \begin{bmatrix} I(p)^{-1/2} & 0 \\ 0 & I(p)^{-1/2} \end{bmatrix} M \begin{bmatrix} I(p)^{-1/2} & 0 \\ 0 & I(p)^{-1/2} \end{bmatrix} = \begin{bmatrix} \omega' & -2\mathrm{i}s \\ -2\mathrm{i}\,\overline{s} & \overline{\omega'} \end{bmatrix}, \tag{6.31}$$

where:

$$\omega':=I(p)^{-1/2}\omega I(p)^{-1/2}\ . \tag{6.32}$$

Then we multiply Eq. (6.31) on the left by $\begin{bmatrix} \mathbf{1} & 0 \\ 2\mathrm{i}\,\overline{s} & \omega' \end{bmatrix}$ and obtain that:

$$\det M=\det I(p)^2\det\bigl(4|s|^2+\omega'\,\overline{\omega'}\bigr). \tag{6.33}$$

We then substitute Eq. (6.33) into Eq. (6.29) and finally obtain (after dropping the primes at ω'):

$$Z_1(\beta,\omega;p)=\frac{\pi^4}{4\beta\det I(p)}\,\mathrm{e}^{\mathrm{tr}[\omega\,I(p)]}\int_0^\infty \frac{\mathrm{d}x\,\mathrm{e}^{-\frac{x}{4\beta}}}{\sqrt{\det\bigl(x+\omega\,\overline{\omega}\bigr)}}. \tag{6.34}$$

The above integral is well defined, because $\det\bigl(x+\omega\,\overline{\omega}\bigr)=\det\bigl(x+\sqrt{\omega}\,\overline{\omega}\sqrt{\omega}\bigr)$ and $\sqrt{\omega}\,\overline{\omega}\sqrt{\omega}$ is strictly positive, since we have assumed that $\det\omega\neq 0$. The generalization of Eq. (6.34) to Bell-diagonal states is straightforward — it is enough to replace $I(p)$ in Eq. (6.30) with the diagonal matrix $4\,\mathrm{diag}(1-p_1-p_2-p_3,p_1,p_2,p_3)$.

Further studies of the integral (6.34) were performed using numerical methods. According to Eq. (6.17) one has to search for a saddle point of $\log Z_1$ with respect to ω. The search was performed by flood-minimizing the Hilbert-Schmidt norm of $\partial\log Z_1(\omega)/\partial\omega_{\alpha\beta}$ (see the sentence below Eq. (2.19), Section 2.2.2 for the definition of the Hilbert-Schmidt norm). For the simplicity we have assumed that $\omega=\mathrm{diag}(\mu,\nu,\nu,\nu)$ and minimized with respect to the parameters $\mu,\nu>0$, paying attention that the obtained minima are not on the border of the region $\omega>0$. The results are presented on Fig. 6.1. We see that for $p\geq 0.89$ the constraints (6.17) can be satisfied. We shall call the interval where it happens the detection region.

Next, the dependence of the average entanglement (6.20) of the continuous ensemble (6.19) on β within the detection region was examined (recall that outside this region the constraints (6.19) are no longer satisfied). Fig. 6.2 shows a sample plot

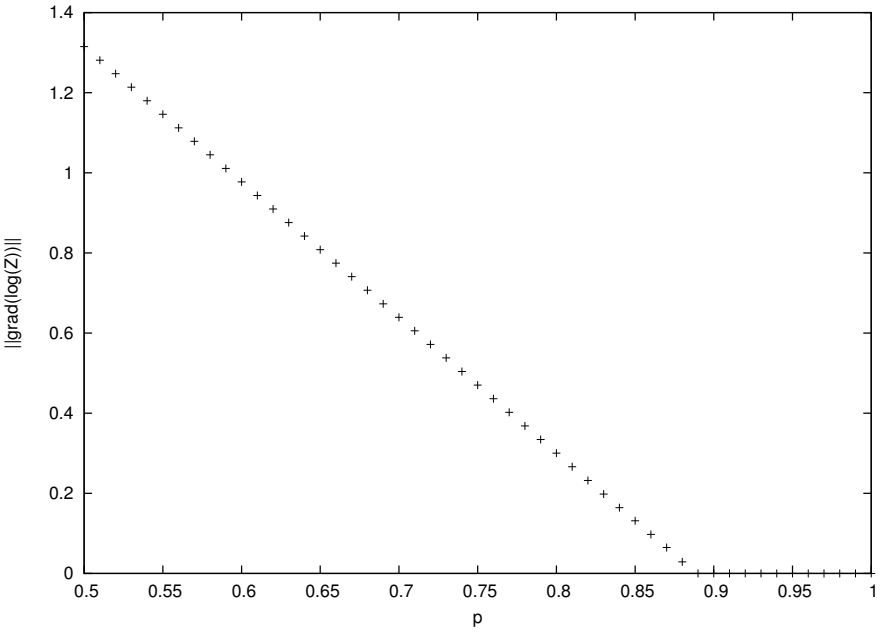

Figure 6.1: The plot of $||\nabla_\omega \log Z_1||_2$ for $\beta = 10$.

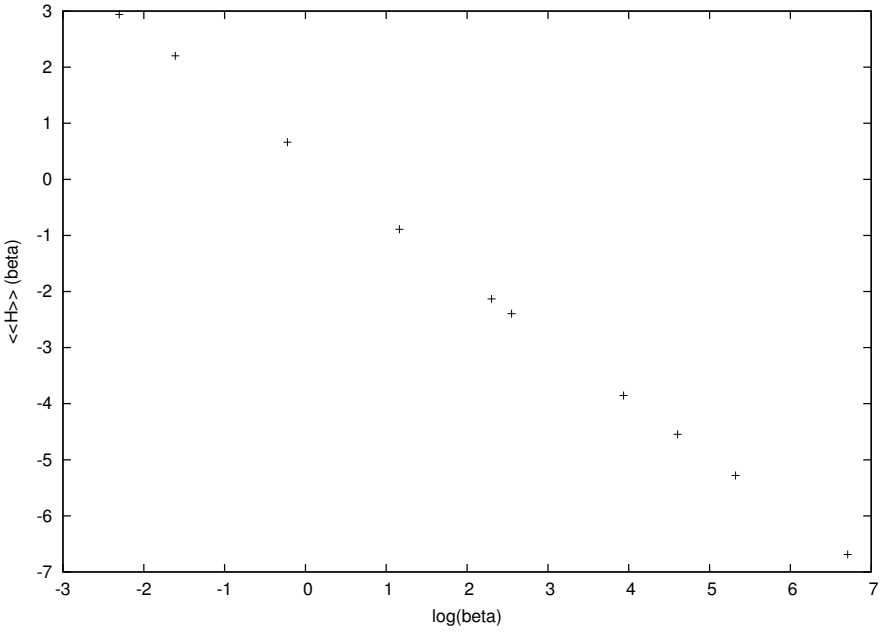

Figure 6.2: The plot of $\langle\langle F_{1\varrho}\rangle\rangle_0$ for $p = 0.90$ on a double log scale.

for $p = 0.9$. One sees that asymptotically the average entanglement indeed vanishes like $1/\beta$. We have also checked that in the limiting case $\beta \to \infty$ the detection region is not altered. Hence, our procedure seems to detect separability of the Werner states (6.21) for $p \geq 0.89$. It misses the separable states with $2/3 \leq p \leq 0.89$ and thus can serve only as a sufficient condition for separability.

It is interesting to note that, quite surprisingly, the same value for p one obtains from the criterion of Braunstein *et al.* [10], which we mentioned at the end of Section 3.2.

6.4 Concluding remarks

Presented statistical mechanical approach to separability problem differs from more traditional techniques in that we studied the space of convex decompositions of a given state, rather than the convex set of all states. Unfortunately, the resulting polynomial equations (6.7) and (6.8) are real and this real structure makes the analysis more complicated than it would be in a complex case. Hence, we applied statistical-mechanical methods to study possible zeros of this system. The justification for the use of statistical methods is still not clear — the basic question being if (or which) separable states possess sufficiently many separable decompositions, i.e. if the solutions of Eq. (6.7) form a set of non-zero measure in $V_{N,r}$.

The application of our method to Werner states (6.21) suggests that at least for separable states in a vicinity of the identity, the partition function shows some qualitative change of behaviour. However, the numerical difficulty already at this simple example was very high and the detection region not very large. One way of improvement of the latter may be to allow for some finite error ϵ in the value of the average entanglement (6.20), fitted in such a way that the detection region is the same as that of the PPT criterion. Then, such gauged, the method could be applied to other states than those of Werner, and again compared with the PPT criterion.

Appendix A

$SU(2)$-characteristic function of the $3 \otimes 3$ Horodecki's state

As an example we calculate for $G = SU(2)$ the characteristic function of the $3 \otimes 3$ PPT entangled state, discovered by Horodecki in Ref. [40]. Since any irreducible representation T of $SU(2) \times SU(2)$ is of the form $T = \tau_{j_1} \otimes \tau_{j_2}$ for some spins j_1, j_2, all we need are the matrix elements $\tau^j_{\mu\nu}$ of the corresponding spin-j representations τ_j of $SU(2)$. The concrete basis $\{|e_\mu\rangle\}$ in which we calculate them is irrelevant for our purposes, as from Eq. (3.7) from Section 3.2 it follows that a change of basis: $\tau_{j_1} \mapsto U_1 \tau_{j_1} U_1^\dagger$, $\tau_{j_2} \mapsto U_2 \tau_{j_2} U_2^\dagger$ induces only a local rotation of the state ϱ:

$$\mathrm{tr}\big[\varrho U_1 \tau_{j_1} U_1^\dagger \otimes U_2 \tau_{j_2} U_2^\dagger\big] = \mathrm{tr}\big[\big(U_1^\dagger \otimes U_2^\dagger \varrho U_1 \otimes U_2\big)\tau_{j_1} \otimes \tau_{j_2}\big], \tag{A.1}$$

and the rotated state $U_1^\dagger \otimes U_2^\dagger \varrho U_1 \otimes U_2$ is separable if and only if ϱ is separable. The above remark concerning bases obviously applies to any kinematical group G.

A convenient formula for $\tau^j_{\mu\nu}$ can be found, for example, in Zhelobenko [112]:

$$\tau^j_{\mu\nu}(g) = \frac{1}{(j-\mu)!} \frac{\mathrm{d}^{j-\mu}}{\mathrm{d}z^{j-\mu}}\bigg|_0 \big[(\alpha z + \beta)^{j-\nu}(-\overline{\beta} z + \overline{\alpha})^{j+\nu}\big], \tag{A.2}$$

where $\mu, \nu = -j, -j+1, \ldots, j$ and α, β are the group parameters:

$$g = \begin{bmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{bmatrix}, \quad |\alpha|^2 + |\beta|^2 = 1. \tag{A.3}$$

From Eq. (A.2) we immediately see that matrix elements of the representation τ_j are homogeneous polynomials of degree $2j$ in the group parameters. Hence, matrix elements of $\tau_{j_1} \otimes \tau_{j_2}$ are polynomilas of bi-degree $(2j_1, 2j_2)$ in (α_1, β_1), (α_2, β_2) as mentioned in Section 3.2 of Chapter 3.

The $3 \otimes 3$ Horodecki's state is given by:

$$\varrho = \frac{1}{8a+1} \begin{bmatrix} a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\ a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+a}{2} & 0 & \frac{\sqrt{1-a^2}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 \\ a & 0 & 0 & 0 & a & 0 & \frac{\sqrt{1-a^2}}{2} & 0 & \frac{1+a}{2} \end{bmatrix}, \tag{A.4}$$

where $0 \leq a \leq 1$. From Eq. (A.2) we find the three dimensional representation of $SU(2)$:

$$\tau_1(g) = \begin{bmatrix} \alpha^2 & -\alpha\overline{\beta} & \overline{\beta}^2 \\ 2\alpha\beta & |\alpha|^2 - |\beta|^2 & -2\overline{\alpha\beta} \\ \beta^2 & \overline{\alpha}\beta & \overline{\alpha}^2 \end{bmatrix}. \tag{A.5}$$

Inserting Eqs. (A.4) and (A.5) into Eq. (3.7), we obtain the characteristic function of the state (A.4):

$$\begin{aligned} \phi_\varrho(g_1, g_2) \;=\; & \frac{a}{8a+1}\Big[(\alpha_1^2 + \frac{1}{2}\overline{\alpha_1}^2)(\alpha_2^2 + \overline{\alpha_2}^2) + (\beta_1\beta_2)^2 \\ & + (\overline{\beta_1\beta_2})^2 + 4\alpha_1\beta_1\alpha_2\beta_2 + 4\overline{\alpha_1\beta_1\alpha_2\beta_2} \\ & + \alpha_1\overline{\beta_1}\alpha_2\overline{\beta_2} + \overline{\alpha_1}\beta_1\overline{\alpha_2}\beta_2 \\ & + (\alpha_1^2 + \overline{\alpha_1}^2)(|\alpha_2|^2 - |\beta_2|^2) \\ & + (|\alpha_1|^2 - |\beta_1|^2)(\alpha_2^2 + \overline{\alpha_2}^2) \\ & + (|\alpha_1|^2 - |\beta_1|^2)(|\alpha_2|^2 - |\beta_2|^2)\Big] \\ & + \frac{\sqrt{1-a^2}}{2}\overline{\alpha_1}^2(\beta_2^2 + \overline{\beta_2}^2) + \frac{1}{2}\overline{\alpha_1}^2(\alpha_2^2 + \overline{\alpha_2}^2). \end{aligned} \tag{A.6}$$

Note that from the fact that the state (A.4) is entangled for $0 < a < 1$, we obtain through Theorem 3.7 from Section 3.3, a highly non-trivial result concerning the function (A.6): the function (A.6) cannot be represented as a convex mixture of products of positive definite functions, depending on parameters (α_1, β_1), and (α_2, β_2) respectively.

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List of Publications

1. J. Korbicz and J. Tafel, *Lagrangian and Hamiltonian for the Bondi-Sachs metrics*, Class. Quant. Grav. **21**, 3301 (2004).

2. J. K. Korbicz, J. I. Cirac, J. Wehr, and M. Lewenstein, *Hilbert's 17th Problem and the Quantumness of States*, Phys. Rev. Lett. **94**, 153601 (2005).

3. J. K. Korbicz, J. I. Cirac, and M. Lewenstein, *Spin Squeezing Inequalities and Entanglement of N Qubit States*, Phys. Rev. Lett. **95**, 120502 (2005).

4. J. K. Korbicz, O. Gühne, M. Lewenstein, H. Häffner, C. F. Roos, and R. Blatt, *Generalized Spin Squeezing Inequalities in N Qubit Systems: Theory and Experiment*, quant-ph/0601038 (submitted to Phys. Rev. A).

5. J. K. Korbicz and M. Lewenstein, *Group-Theoretical Approach to Entanglement*, quant-ph/0601189 (submitted to Phys. Rev. A).

6. J. K. Korbicz and M. Lewenstein, quant-ph/0603082, *Remark on a Group-Theoretical Formalism for Quantum Mechanics and the Correspondence Principle*, (submitted to Found. Phys. Lett.).

7. A. Kubasiak, J. K. Korbicz, J. Zakrzewski, and M. Lewenstein, *Fermi-Dirac Statistics and the Number Theory*, Europhys. Lett. **72**, 506 (2005).

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