Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

# The Quest for Three-Partite Marginal Quantum Non-Locality and a Link to Contextuality

Master Thesis

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August 27, 2012

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**Abstract**

We report on the progress made towards finding non-local behaviour in the bipartite reduced states of a three-partite quantum state. In particular we investigate the W and Aharonov state, which have symmetric bipartite reduced states. To this end we present computational methods. We also show that a maximally non-local bipartite quantum behaviour can be constructed from any Kochen-Specker set, thus showing a very close link between contextuality and non-locality.

**Acknowledgements**

I would like to express my gratitude towards Stefan Wolf for warmly welcoming me in Lugano and the insightful and helpful discussions during the course of this thesis. I thank Marcel Pfaffhauser for his enduring support and advice, as well as Daniela Frauchiger for sharing her insights into Physics and the surrounding mountains. I also would like to thank Christian Badertscher and Ämin Baumeler for their helpful comments and suggestions. Last but not least I thank my family for their support.

# Contents

Chapter 1

# Introduction

> *"I think I can safely say that nobody understands quantum mechanics."*
>
> — Richard Feynman, *The Character of Physical Law*

Even though Quantum Theory may be seen as an extension of classical probability theory [16, 25, 41], its place as a physical theory does not fail to challenge our perception of reality.

One aspect of Quantum Theory, in contrast to classical theories, is the inseparability of states in composite systems, a property known as *entanglement*.

Physical systems whose joint state space may be described as a quantum mechanical composite of spaces may surprisingly be physically separated even if the joint quantum mechanical state is not separable, but is entangled. This leads to peculiar situations where physical systems are separable, whereas their quantum mechanical descriptions are not.

Furthermore, it is possible to conduct local measurements on such physically separated systems so that the quantum mechanically expected outcomes are correlated but not predictable. This was eloquently noted by Einstein, Podolski and Rosen (EPR) in their 1935 paper "Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?" [15]. They raise the question whether a more complete description of physical reality addressing this peculiarity may be found.

Responding to EPR, in 1964, John Bell [8] showed that no "hidden variable" interpretation of Quantum Mechanics, a class of extensions to the theory, is compatible with quantum mechanical predictions . He showed this by deriving inequalities that must be satisfied for all behaviours that are separable given some shared hidden variables and demonstrating the existence of quantum mechanical behaviours that lead to a violation of these inequalities. Such behaviours are called *non-local*.

We are left with the situation where there exist separable physical systems with non-separable quantum mechanical descriptions and also non-separable (non-local) quantum mechanical behaviours.

In this thesis we investigate which quantum states admit non-local behaviour. In particular we are interested in bipartite quantum states that are the marginal of three-partite states. We call this *three-partite marginal quantum non-locality*. To this end, we describe various computational methods for studying behaviours. We also prove certain characteristics of the space of local behaviours and show a close link between contextuality and non-locality.

## 1.1 Overview

The thesis is structured as follows. We begin by stating fundamental results from Linear Algebra, the study of convex sets and the basic concepts of Quantum Mechanics.

We proceed, in Chapter 3, by introducing probabilistic behaviours, properties of such behaviours and a hierarchy. Here we also prove certain characteristics of local behaviours and the space they are contained in.

Chapter 4 discuses the non-locality of Quantum Mechanics. We review the results by Werner. Further, we show a close link between contextuality and non-locality by proving that a bipartite quantum behaviour which maximally violates a Bell inequality can be constructed from any Kochen-Specker set.

In order to investigate non-local behaviours we present in Chapter 5 various computational methods used previously for similar studies and in the context of Polyhedral Computation.

In Chapter 6, we describe the setting of three-partite marginal quantum non-locality and report on the progress made towards finding such states and behaviours.

We conclude with a discussion of the topics addressed and briefly mention possible directions for future inquiry.

Chapter 2

# Preliminaries

## 2.1 Linear Algebra

In the following, we briefly state fundamental concepts from standard Linear Algebra that will be used to discuss the main topics. For a more rigorous and complete treatment see Artin [3], Connell [12] or the introductory sections on Linear Algebra in Nielsen and Chuang [36].

### 2.1.1 Vector space

A vector space $V$ over a field $F$ is a set together with addition and scalar multiplication, satisfying certain condition.

We will mostly use vector spaces over real numbers, the set of all $n$-vectors, which we will denote as $\mathbb{R}^n$. The zero vector $(0, 0, \ldots, 0) \in \mathbb{R}^n$ will be denoted as 0.

Let $(v_1, v_2, \ldots, v_n)$ be an ordered set of elements of $V$. A linear combination of $(v_1, v_2, \ldots, v_n)$ is any vector

$$w = c_1 \cdot v_1 + c_2 \cdot v_2 + \ldots + c_n \cdot v_n$$

where $c_i \in F$.

The set of all vectors $w$ which are linear combinations of $(v_1, v_2, \ldots, v_n)$ form a subspace $W$ of $V$, called the subspace spanned by the set.

A set of vectors $(v_1, v_2, \ldots, v_n)$ is *linearly independent* if and only if

$$c_1 \cdot v_1 + c_2 \cdot v_2 + \ldots + c_n \cdot v_n = 0$$

implies that all coefficients $c_i = 0$. Conversely, a set of vectors is called *linearly dependent* if and only if there exists a non-zero coefficient $c_i$.

If the space spanned by a set of linear independent vectors $B = (b_1, b_2, \ldots, b_k)$ is $V$, then $B$ is called a *basis* of $V$.

The *dimension* of $V$ is the number of vectors in a basis $B$ of $V$.

### 2.1.2 System of linear equations

A system of linear equations may be written in the form $Ax = b$.

A system of linear equations is *homogeneous* if $b$ is the zero vector $Ax = 0$.

The space of solution vectors $x$ is the *null space* of $A$, denoted as $\text{null}(A)$. The dimension of the null space is called the nullity of $A$.

The *rank* of $A$ is the number of linearly independent rows.

By the *rank-nullity theorem* we have the following relation

$$\text{rank}\, A + \text{nullity}\, A = \dim V.$$

There is a close relationship between the solutions to a non-homogeneous and homogeneous system. If $p$ is a solution to the homogeneous system $Ap = b$, then the set of solutions to $Ax = b$ is $\{p + v \mid v \in \text{null}(A)\}$. Note that this solution set is in general not a vector space, it is an *affine subspace* of $V$.

### 2.1.3 Hyperplane

A hyperplane $(z, z_0)$ of an $n$ dimensional space is a $n-1$ dimensional subspace defined by a single linear equality

$$z^\top x = z_0. \tag{2.1}$$

In general the subspace is affine. If $z_0 = 0$ it is also a vector subspace.

This affine space separates the space into two half-spaces that are given by the inequalities

$$z^\top x < z_0$$

and

$$z^\top x > z_0.$$

Note that linear equalities (and thus hyperplanes) may be arbitrary scaled. For example

$$cz^\top x = cz_0$$

defines the same subspace as (2.1) for any scalar $c$.

## 2.2 Convex Sets and Polytopes

Many concepts discussed in the following chapters may be elegantly described by convex sets and polytopes. In this section we provide a brief overview of definitions and important results from the study of such objects. For a more complete treatment we refer the reader to Ziegler [57] and Lauritzen [32], from where we take the material presented here.

### 2.2.1 Convex set

**Definition 2.1 (Convexity)** *A set $K \subset \mathbb{R}^d$ is* convex *if and only if $a, b \in K$ and $0 \leq \lambda \leq 1$ imply $\lambda a + (1-\lambda)b \in K$.*

**Definition 2.2 (Convex hull)** *Let $v_1, v_2, \dots, v_n \in \mathbb{R}^d$ be a finite set of vectors, then we define the* convex hull

$$\begin{aligned}&\operatorname{conv}(v_1, v_2, \dots, v_n) := \\ &\qquad \{\lambda_1 v_1 + \lambda_2 v_2 + \dots + \lambda_n v_n \mid \lambda_1, \dots, \lambda_n \geq 0, \lambda_1 + \dots + \lambda_n = 1\}.\end{aligned}$$

It follows straightforwardly that the convex hull is a convex set.

### 2.2.2 Polytopes

**Definition 2.3 (Polytopes)** *A polytope is the convex hull of a finite set of points in $\mathbb{R}^d$.*

From the Minowsky-Weyl Theorem an equivalent way of describing polytopes follows:

**Theorem 2.4 (Halfspace representation of polytopes)** *$\mathcal{P}$ is a polytope if and only if there exists a system of finitely many linear inequalities so that*

$$\mathcal{P} = \left\{ x \in \mathbb{R}^d \mid Ax \leq b \right\}.$$

For a proof the reader is referred to Ref. [57, Theorem 1.1].

This allows us to represent polytopes as the intersection of a finite number of linear inequalities; we will call this representation *halfspace representation*.

**Proposition 2.5 (Unique closest point)** *Let $\mathcal{P} \subset \mathbb{R}^d$ be a polytope and $z \in \mathbb{R}^d$. Then there exists an unique point $r \in \mathcal{P}$ such that*

$$\|z - r\| = \min \left\{ \|z - r'\| \mid r' \in \mathcal{P} \right\}.$$

The claim follows from Ref. [32, Corollary 3.0.2].

## 2.3 Quantum Mechanics

For the sake of completeness, we state the postulates of Quantum Mechanics and discuss key concept such as density operators, entanglement and generalized measurements (POVM).

The following section follows the lines of Nielsen and Chuang [36] and Renner [46].

### 2.3.1 The postulates of Quantum Mechanics

**States** Associate to any isolated system is a Hilbert space $\mathcal{H}$ known as the *state space*. The system is completely described by a normalized vector $\varphi \in \mathcal{H}$, the *state vector*.

**Composition** For two systems with state space $\mathcal{H}_A$ and $\mathcal{H}_B$, the state space of the product system is $\mathcal{H}_A \otimes \mathcal{H}_B$. Furthermore, if the individual systems are in states $\varphi_A \in \mathcal{H}_A$ and $\varphi_B \in \mathcal{H}_B$, then the joint state is

$$\varphi_A \otimes \varphi_b \in \mathcal{H}_A \otimes \mathcal{H}_B$$

.

**Evolution** The evolution of an isolated system with state space $\mathcal{H}$ is described by a unitary transformation. That is, a state $\varphi \in \mathcal{H}$ is related to the post-evolution state $\varphi' \in \mathcal{H}$ by an unitary operator $U$:

$$\varphi' = U\varphi$$

.

**Measurements** A (projective) measurement is described by an *observable* $M$, a Hermitian operator on the state space of the system being observed. Each eigenvalue $x$ of $M$ corresponds to a possible measurement outcome. If the system is in state $\varphi \in \mathcal{H}$, then the probability of observing outcome $x$ is given by

$$p(x) = \operatorname{tr}\left(P_x |\varphi\rangle\langle\varphi|\right)$$

where $P_x$ denotes the projector onto the eigenspace belonging to the eigenvalue $x$. The state $\varphi'$ of the system after observing $x$ is

$$\varphi' = \sqrt{\frac{1}{p(x)}} P_x \varphi.$$

### 2.3.2 Density operators

Often it is not enough to consider isolated quantum systems. We use the notion of density operators which is able to represent the state of a system that is, in general, not isolated.

**Definition 2.6 (Density operator)** *A* density operator $\rho$ *on a Hilbert space* $\mathcal{H}$ *is a normalized positive operator on* $\mathcal{H}$*, i.e.* $\rho \geq 0$ *and* $\mathrm{tr}(\rho) = 1$*. The set of density operators on* $\mathcal{H}$ *is denoted by* $\mathcal{S}(\mathcal{H})$*. A density operator is said to be* pure *if it has the form* $\rho = |\varphi\rangle\langle\varphi|$*. A density operator that is not pure is called* mixed*. If* $\mathcal{H}$ *is d-dimensional and* $\rho$ *has the form* $\rho = \frac{1}{d}I$ *then it is called* fully mixed.

It follows from the spectral decomposition theorem that any density operator can be written in the form

$$\rho = \sum_x \lambda_x |e_x\rangle\langle e_x|$$

where $\lambda_x$ are the eigenvalue of $\rho$ and $e_x$ the corresponding eigenvectors.

The postulates of Quantum Mechanics may be stated in the language of density operators:

**State** The state of a system is represented as a density operator on a state space $\mathcal{H}$. For an isolated system whose state is $\varphi \in \mathcal{H}$ the corresponding density operator is defined by $\rho = |\varphi\rangle\langle\varphi|$.

**Composition** The state of a composite system with state spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ is represented as density operator on $\mathcal{H}_A \otimes \mathcal{H}_B$. Furthermore, if the individual systems are in states $\rho_A \in \mathcal{S}(\mathcal{H}_A)$ and $\rho_B \in \mathcal{S}(\mathcal{H}_B)$, then the joint state is $\rho_A \otimes \rho_B \in \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$.

**Evolution** Any isolated evolution of a system corresponds to a unitary on the state space $\mathcal{H}$. That is, a state $\rho \in \mathcal{S}(\mathcal{H})$ is related to the post-evolution state $\rho' \in \mathcal{S}(\mathcal{H})$ by and unitary operator $U$:

$$\rho' = U\rho U^\dagger$$

.

**Measurements** A (projective) measurement is described by an observable $M$, a Hermitian operator on the state space of the system being observed. Each eigenvalue $x$ of $M$ corresponds to a possible measurement outcome. If the system is in state $\rho \in \mathcal{S}(\mathcal{H})$, then the probability of observing outcome $x$ is given by

$$p(x) = \mathrm{tr}\,(P_x \rho)$$

where $P_x$ denotes the projector onto the eigenspace belonging to the eigenvalue $x$. The state $\rho'$ of the system after observing $x$ is

$$\rho' = \frac{1}{p(x)} P_x \rho P_x.$$

### 2.3.3 Partial trace and purification

Let $\mathcal{H}_A \otimes \mathcal{H}_B$ be a composite quantum system which is in a state $\rho_{AB} = |\Psi\rangle\langle\Psi|$ for some $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. Following from the properties of the partial trace and the postulates, the *reduced state* $\rho_A = \mathrm{tr}_B(\rho_{AB})$ fully characterizes all observable properties of the subsystem $\mathcal{H}_A$.

Note that the reduced state $\rho_A$ of a pure joint state $\rho_{AB}$ is not necessarily pure.

Conversely, any mixed density operator $\rho_A$ can be seen as part of a pure state on a larger system, there exists a pure density operator $\rho_{AB}$ on a joint system $\mathcal{H}_A \otimes \mathcal{H}_B$ such that

$$\rho_A = \mathrm{tr}_B\, \rho_{AB}.$$

Such a state $\rho_{AB}$ is called a *purification* of $\rho_A$.

### 2.3.4 Entanglement

The following definition of separability and entanglement of density operators is due to Werner [56] (then called classically correlated and EPR correlated).

**Definition 2.7 (Separability)** *A density operator $\rho \in \mathcal{S}\left(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_n\right)$ is called* separable *if it can be written as a convex combination of product states*

$$\rho = \sum_i p_i \rho_1^i \otimes \rho_2^i \otimes \cdots \otimes \rho_n^i$$

*where $\rho_j^i \in \mathcal{S}\left(\mathcal{H}_j\right)$.*

**Definition 2.8 (Entanglement)** *A density operator $\rho$ is called* entangled *if it is not separable.*

The *positive partial transpose (PPT) criterion* is a necessary condition for the separability of a density operator [38].

For systems of dimension $2 \times 2$ and $2 \times 3$ it has been shown that the PPT criterion is not only a necessary but also a sufficient condition for separability [27]. Thus it is a complete characterization of entanglement in those cases.

In general, it is hard to decide whether a given state is separable or entangled, this is called the separability problem or entanglement detection problem [23].

For an extensive review of topics related to quantum entanglement the reader is referred to Horodeckis [29].

### 2.3.5 Generalized measurements

In the most general form measurements on quantum systems may be expressed as *Positive Operator-Valued Measure (POVM)*.

Let $\{F_x\}$ be a set of positive operators such that $\sum_x F_x = I$. The operators $F_x$ are known as *POVM elements*. The complete set $\{F_x\}$ is known as *POVM*.

The probability of observing outcome $x$ is given by

$$p(x) = \mathrm{tr}(F_x \rho).$$

Note that projective measurements, as described above, are a special case of POVM measurements.

Chapter 3

# Probabilistic Behaviours

## 3.1 Probabilistic Behaviours

Generally, the behaviour of a $k$-partite input-output system, where the parties choose an input $a_i$ and receive and output $x_i$, may be described as a probability distribution

$$P\left(x_1, x_2, \ldots, x_k \mid a_1, a_2, \ldots, a_k\right)$$

giving the probability of observing outputs $x_1, \ldots, x_k$ for inputs $a_1, \ldots, a_k$.

In the following, we will assume that the inputs and outputs for all parties take values from a finite alphabet $a_i \in \{0, \ldots, n-1\}$ and $x_i \in \{0, \ldots, m-1\}$, we will refer to such behaviours as $(n, m)$*-behaviours*.

As we will be mostly considering the bipartite case ($k = 2$), we will use the notation: $x = x_1$, $y = x_2$, $a = a_1$ and $b = a_2$, corresponding to Alice and Bob. The probability distribution describing the bipartite behaviour is then

$$P\left(x, y \mid a, b\right).$$

When considering three-partite systems, we identify $z = x_3$ and $c = a_3$, calling the third party Charlie.

A probabilistic behaviour $P\left(x_1, x_2, \ldots, x_k \mid a_1, a_2, \ldots, a_k\right)$ may be written as a vector $p \in \mathbb{R}^{n^k \cdot m^k}$ with elements

$$p_{x_1,\ldots,x_k,a_1,\ldots,a_k} = P\left(x_1, x_2, \ldots, x_k \mid a_1, a_2, \ldots, a_k\right). \tag{3.1}$$

However, not every $p \in \mathbb{R}^{n^k \cdot m^k}$ corresponds to a behaviour.

A vector $p$ is a probabilistic behaviour if and only if it satisfies the *normalization conditions*

$$\sum_{x_1,\ldots,x_k} p_{x_1,\ldots,x_k,a_1,\ldots,a_k} = 1 \tag{3.2}$$

for all $a_1, \ldots, a_k$ and the *non-negativity conditions*

$$p_{x_1,\ldots,x_k,a_1,\ldots,a_k} \geq 0 \tag{3.3}$$

for all $x_1, \ldots, x_k, a_1, \ldots, a_k$.

By stating these conditions explicitly we gain insight into the space of behaviours. The normalization conditions may be seen as a non-homogeneous system of $n^k$ linearly independent equalities. The space of normalized vectors is an affine subspace of $\mathbb{R}^{n^k \cdot m^k}$ with dimension $n^k \cdot m^k - n^k$.

The non-negativity conditions, on the other hand, define half-spaces. The intersection of these half-spaces with the normalized vectors is a convex polytope, i.e. the set of probabilistic behaviours forms a convex polytope.

When appropriate, we will represent a bipartite $(n, m)$-behaviour as a $(nm \times nm)$-matrix

$$\begin{pmatrix} P(0,0 \mid 0,0) & P(0,1 \mid 0,0) & \cdots & P(0,m-1 \mid 0,n-1) \\ P(1,0 \mid 0,0) & P(1,1 \mid 0,0) & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ P(m-1,0 \mid n-1,0) & \cdots & \cdots & P(m-1,m-1 \mid n-1,n-1) \end{pmatrix}.$$

## 3.2 Non-Signaling

**Definition 3.1 (Non-signaling)** *A k-partite $(n, m)$-behaviour is* non-signaling, *when the marginal distribution for every subset of parties $\{i_1, i_2, \ldots, i_l\}$ only depends on its corresponding inputs*

$$P(x_{i_1}, x_{i_2}, \ldots, x_{i_l} \mid a_1, a_2, \ldots, a_k) = P(x_{i_1}, x_{i_2}, \ldots, x_{i_l} \mid a_{i_1}, a_{i_2}, \ldots, a_{i_l}). \tag{3.4}$$

This corresponds to behaviours where any subset of the $k$ parties are not able to gain information on the input of other parties. In other words, behaviours that can not be used to communicate or signal, thus *non-signaling*.

As shown in Ref. [6] all conditions of form (3.4) follow from the conditions

$$\begin{aligned} &\sum_{x_i} P(x_1, \ldots, x_i, \ldots, x_k \mid a_1, \ldots, a_i, \ldots, a_k) \\ = &\sum_{x_i} P\left(x_1, \ldots, x_i, \ldots, x_k \mid a_1, \ldots, a_i', \ldots, a_k\right) \end{aligned} \tag{3.5}$$

for all $i$, pairs $(a_i, a_i')$, $x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_k$ and $a_1, \ldots, a_{i-1}, a_{i+1}, \ldots, a_k$.

The non-signaling conditions may be seen as a homogeneous system of $k\binom{n}{2}m^{k-1}n^{k-1}$ linear equalities $C^{\text{ns}}p = 0$. We will refer to the solution space of this system, i.e. $\mathrm{null}(C^{\mathrm{ns}})$, as the *non-signaling vector subspace* $\mathcal{V}^{\mathrm{ns}}$. A basis of this space will be called $B^{\mathrm{ns}}$.

Note, however, that the non-signaling vector subspace is not the space of non-signaling behaviours as the vectors may not satisfy the normalization or non-negativity conditions. The space of all non-signaling probabilistic behaviours is in fact a polytope [34] which is called the *non-signaling polytope* $\mathcal{P}^{\mathrm{ns}}$.

## 3.3 Locality

An important class of behaviours we will study are the local behaviours. These are behaviours where the joint behaviour of the parties may be decomposed into single party behaviours given some shared random value, often called *hidden variables*.

**Definition 3.2 (Local behaviour)** *A bipartite behaviour is* local *if and only if it can be decomposed as*

$$P\left(x,y \mid a,b\right) = \int_{\lambda} P\left(x \mid a,\lambda\right) P\left(y \mid b,\lambda\right) P(\lambda) d\lambda \tag{3.6}$$

*for some range of values $\lambda \in \Lambda$.*

The term locality comes from the physical interpretation of such behaviours for (physically) separable parties. Mathematically it is a separability criterion.

Observe that all local behaviours are non-signaling as the marginal distributions for both parties only depend on their corresponding inputs. The converse, however, does not hold.

### 3.3.1 Local polytope

We will only consider bipartite behaviours with finite input and output alphabet. The space of such local behaviours may be characterized as a polytope. This is a well known result and has been stated by various authors [18,39,55]. Nevertheless, given the importance of this result, we give a proof of this statement.

First, we define a special class of local behaviours.

**Definition 3.3 (Local deterministic behaviours)** *A* local deterministic behaviour *(*ldb*) $P^{ldb}\left(x,y \mid a,b\right)$ is a $(n,m)$-behaviour with*

$$P^{ldb}\left(x,y \mid a,b\right) = P_s(x \mid a) P_{s'}(y \mid b) \tag{3.7}$$

*where $P_s(x \mid a)$ and $P_{s'}(y \mid b)$ are deterministic probability distributions that may be written as*

$$P_s(x \mid a) = \delta_{s_a,x} \quad P_{s'}(y \mid b) = \delta_{s'_b,y}$$

*for some strings $s, s' \in \{0, \dots, m-1\}^n$, with $\delta_{i,j}$ being the Kronecker delta function.*

The string $s, s'$ are the *local deterministic strategies*, functions $s, s' : \{0, \dots, n-1\} \to \{0, \dots, m-1\}$ assigning a deterministic outcome for every input.

As the number of such strategies is finite for fixed $n$ and $m$, the number of different local deterministic behaviours is $m^{2n}$.

We will label the local deterministic behaviours either with arbitrary indices, e.g. $P_i^{\mathrm{ldb}}(x, y \mid a, b)$, or alternatively by the defining local deterministic strategies, e.g. $P_{s,s'}^{\mathrm{ldb}}(x, y \mid a, b)$.

**Proposition 3.4** *A local bipartite behaviour with finite input and output alphabet (e.g. a $(n, m)$-behaviour) can be decomposed as a convex combination of the local deterministic behaviours*

$$P(x, y \mid a, b) = \sum_i P_i^{ldb}(x, y \mid a, b)\, c_i \tag{3.8}$$

*where $c_i$ are the coefficients of a convex combination ($c_i \geq 0$ and $\sum_i c_i = 1$).*

**Proof** Consider the local behaviour

$$P(x, y \mid a, b) = \int_\lambda P(x \mid a, \lambda)\, P(y \mid b, \lambda)\, P(\lambda) d\lambda \tag{3.9}$$

with finite input and output alphabet. Observe that any finite distribution $P(x \mid a, \lambda)$ may be written as a convex combination of deterministic probability distributions

$$P(x \mid a, \lambda) = \sum_s P_s(x|a) \alpha_s^\lambda \tag{3.10}$$

where the coefficients $\alpha_s^\lambda$ of the convex combination depend on $\lambda$.

By replacing terms, we get

$$\begin{aligned} P(x, y \mid a, b) &= \int_\lambda \left( \sum_s P_s(x|a) \alpha_s^\lambda \right) \left( \sum_{s'} P_{s'}(y|b) \beta_{s'}^\lambda \right) P(\lambda) d\lambda \\ &= \sum_{s,s'} P_s(x|a) P_{s'}(y|b) \int_\lambda \alpha_s^\lambda \beta_{s'}^\lambda P(\lambda) d\lambda. \end{aligned}$$

We set $c_{s,s'} = \int_\lambda \alpha_s^\lambda \beta_{s'}^\lambda P(\lambda) d\lambda$ and observe that $P_s(x|a) P_{s'}(y|b)$ correspond to the local deterministic behaviours, arriving at

$$P(x, y \mid a, b) = \sum_{s,s'} P_{s,s'}^{\mathrm{ldb}}(x, y \mid a, b)\, c_{s,s'}.$$

It follows from the fact that $P(\lambda)$ is a probability distribution that $c_{s,s'}$ are indeed coefficients of a convex combination, thus proving the claim. $\square$

From Proposition 3.4 and the fact that there are a finite number of local deterministic behaviours we have that the set of local $(n, m)$-behaviours is a polytope with the local deterministic behaviours as extremal points.

**Definition 3.5 (Local polytope)** *The space of local $(n, m)$-behaviours is a polytope with the local deterministic behaviours as extremal points. This polytope is called the* local polytope $\mathcal{P}^{local}_{n,m}$. *When appropriate we simply write $\mathcal{P}^{local}$.*

#### Diameter of local polytope

We are able to state the diameter of the local polytope, i.e. the maximal distance between any two points in the polytope.

**Proposition 3.6 (Diameter of local polytope)** *The maximal (euclidean) distance between any two points in the local polytope is*

$$\max_{p,p' \in \mathcal{P}^{local}} (\|p - p'\|) = \sqrt{2}n.$$

**Proof** Observe that the maximal euclidean distance between any two probabilistic behaviours is attained when the behaviours are deterministic and the supports are non-overlapping. Let $p$ an $p'$ be two such behaviours. As $(p - p')$ only contains non-zero elements with value $\pm 1$ and there are exactly $n^2$ values 1 and $n^2$ values $-1$ (for every possible input pair). We have

$$\|p - p'\|^2 = (p - p')^\top (p - p') = 2n^2.$$

Now to show that there exist deterministic $p, p' \in \mathcal{P}^{\text{local}}$ with non-overlapping support. Consider the local deterministic behaviours $p = p^{\text{ldb}}_{s,s'}$ and $p' = p^{\text{ldb}}_{\bar{s},s'}$ where $\bar{s}$ is the string with $s_a = 1 \Leftrightarrow \bar{s}_a = 0$. As can be easily verified $p$ and $p'$ have non-overlapping support and thus maximal distance between them, proving the claim. $\square$

### 3.3.2 Bell inequalities

There exist linear inequalities where all local behaviours are on one side of the hyperplane defined by the inequality. We call such inequalities *Bell inequalities.*

**Definition 3.7 (Bell inequality)** *A hyperplane $(z, z_0)$ is called a Bell inequality if and only if*

$$z^\top p - z_0 \leq 0 \text{ for all } p \in \mathcal{P}^{local}.$$

Note that there exists trivial Bell inequalities which do not separate the space of behaviours we are interested in. We define a special class of Bell inequalities which are of greater interest.

**Definition 3.8 (Non-trivial Bell inequality)** *A Bell inequality is non-trivial if and only if there exists a point $p^{ns} \in \mathcal{P}^{ns}$ so that*

$$z^\top p^{ns} - z_0 > 0.$$

The number of Bell inequalities is not finite. However, from the halfspace representation of polytopes we have that there exists a finite set of Bell inequalities that fully define the polytope. A minimal set of such inequalities corresponds to the faces of the polytope.

### 3.3.3 Multipartite non-locality

Definition 3.2 of local behaviours can be straightforwardly generalized for $k$-partite behaviours. The space of such behaviours is also a polytope with diameter $\sqrt{2}n^{k/2}$ which can be seen by generalizing propositions 3.4 and 3.6.

However, as noted by Svetlichny [51], there exist three-partite behaviours that are non-local, i.e. can not be decomposed as

$$P\left(x,y,z \mid a,b,c\right) = \int_\lambda P\left(x \mid a,\lambda\right) P\left(y \mid b,\lambda\right) P\left(z \mid c,\lambda\right) P(\lambda) d\lambda \tag{3.11}$$

but may be written as

$$\begin{aligned} P\left(x,y,z \mid a,b,c\right) = & q_1 \int_\lambda P\left(x,y \mid a,b,\lambda\right) P\left(z \mid c,\lambda\right) P(\lambda) d\lambda \\ & + q_2 \int_\mu P\left(x,z \mid a,c,\mu\right) P\left(y \mid b,\mu\right) P(\mu) d\mu \\ & + q_3 \int_\nu P\left(y,z \mid b,c,\nu\right) P\left(x \mid a,\nu\right) P(\nu) d\nu \end{aligned} \tag{3.12}$$

where $q_1, q_2, q_3$ are coefficients of a convex combination.

Such behaviours are not *genuinely three-partite non-local* as they may be decomposed into bipartite non-local behaviours.

Svetlichny derived an inequality which holds for all behaviours of form (3.12) and showed that there are quantum mechanical behaviours that violate this inequality. Showing that quantum behaviours can be genuinely three-partite non-local.

The space of non-signaling behaviours of form (3.12) for finite input and output alphabet can be shown to be a polytope with extremal points being combinations of points in the two-partite non-signaling polytope and one-partite local deterministic behaviours.

The general case of genuine $k$-partite non-locality has been studied [7] and quantum behaviours have been shown to be genuinely $k$-partite non-local [4].

## 3.4 Quantum Behaviour

**Definition 3.9 (Quantum behaviour)** *We call a behaviour quantum, if the behaviour can be written as*

$$P\left(x_1, x_2, \ldots, x_k \mid a_1, a_2, \ldots, a_k\right) = \operatorname{tr}\left(F_{x_1}^{a_1} \otimes \cdots \otimes F_{x_k}^{a_k} \rho\right)$$

*where $\rho$ is a quantum state and $\{F_{x_j}^{a_k}\}_{x_j}$ are sets of POVM operators.*

*The space of all possible quantum behaviours is $\mathcal{C}^{\mathrm{Q}}$. The space of all quantum behaviours using the state $\rho$ is $\mathcal{C}_\rho^{\mathrm{Q}}$.*

In the following we will, if not otherwise noted, restrict ourselves to projective measurements which represent a special case of POVM measurements (see Section 2.3.5).

It follows from the separability of the measurement operators and the partial trace that all quantum behaviours are non-signaling. However, as first shown by Bell [8], not all quantum behaviours are local.

## 3.5 Hierarchy of Behaviour

We have following hierarchy of bipartite behaviours:

$$\mathcal{P}^{\text{local}} \subsetneq \mathcal{C}^{\mathrm{Q}} \subseteq \mathcal{P}^{\text{ns}} \subsetneq \mathcal{V}^{\text{ns}} \subsetneq \mathbb{R}^{n^2 \cdot m^2}. \tag{3.13}$$

Note that for $(2,2)$-behaviours we have strict inclusion of $\mathcal{C}^{\mathrm{Q}}$ in $\mathcal{P}^{\text{ns}}$ (this is known as Tsirelson's bound [54]). However, it is unclear if there is strict inclusion in general.

Considering the non-signaling vector space $\mathcal{V}^{\text{ns}}$ may seem unintuitive and unnecessary, but as we shall see, it will be useful for studying computational methods.

Chapter 4

# Quantum Non-Locality

## 4.1 Quantum States Admitting Non-Local Behaviour

It is clear that the behaviours of separable states are local, i.e. do not admit non-local behaviour. However, the converse, that all non-separable (entangled) states admit non-local behaviour, is not true.

For pure states, it has been shown by Gisin [20] and Gisin and Peres [21] that all bipartite entangled pure states admit non-local behaviour. Furthermore, Popescu and Rohrlich were able to show that all multipartite entangled pure states admit non-local behaviour [44].

The situation for mixed states, however, is more complicated. There exists entangled mixed states that do not admit non-local behaviour. A general classification whether a state admits non-local behaviour is unknown. In fact, deciding whether a state $\rho$ admits non-local behaviour is a central topic we address in Chapter 6.

In the following we briefly discuss an important result regarding non-locality of mixed states by Werner.

### 4.1.1 Werner states

Werner [56] showed that for a certain class of bipartite entangled mixed states any projective measurements always give a local behaviour, by constructing a local hidden variable model for any set of measurements.

The generalized class of such states [5] is given by an operator on a composite of two $d$ dimensional spaces $\mathcal{H}_d \otimes \mathcal{H}_d$

$$\rho = \alpha \frac{2P^{\text{anti}}}{d(d-1)} + (1-\alpha)\frac{I}{d^2} \tag{4.1}$$

where $I$ is the identity, $P^{\text{anti}} = \frac{I - \sum_{i,j} |ij\rangle\langle ji|}{2}$ and some parameter $\alpha$.

For $\alpha > \frac{1}{1+d}$ the state $\rho$ is entangled.

The states for which Werner constructed a local model have $\alpha = \frac{d-1}{d}$.

In the case $d = 2$ the states are mixtures of the singlet $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ and the fully mixed state

$$\rho = \alpha|\psi^-\rangle\langle\psi^-| + (1-\alpha)\frac{I}{4}.$$

For $d = 2$ it is also known that states with $\alpha > 1/\sqrt{2}$ violate the CHSH inequality [28, 38].

Barrett [5] was able to extend the local hidden variable model to generalized measurement (POVM) for

$$\alpha = \frac{1}{d+1}(d-1)^{d-1}d^{-d}(3d-1)$$

which for $d = 2$ evaluates to $\alpha \approx 0.416$.

### 4.1.2 Hidden non-locality

Even though bipartite entangled states may not admit non-local behaviour, Popescu [42] discovered that certain Werner states allow quantum teleportation, a process where a quantum state at an input system is obtained at a remote output system, while the two systems may only use classical communication and a pre-shared quantum state.

Extending this result, it was shown possible to achieve non-local behaviour with Werner states (of dimension $\geq 5$) by applying sequential measurements [43].

Peres [37] showed that if not only a single copy of a state is allowed, but multiple copies are shared, then non-local behaviour can be achieved from a larger set of states by sequential measurements.

These results are not in contradiction to Werner's result. The relation between local hidden variable models and sequential measurements has been studied by Zukowski et al. [58] and Teufel et al. [53].

The hypothesis that all entangled quantum states can show non-local behaviour for sequential measurements seems natural and has been explicitly raised by Barrett [5, Hypothesis 2]. However, the hypothesis remains unknown.

## 4.2 From Contextuality to Non-locality

In 1968, Kochen and Specker [31] showed that any hidden variable model, which is compatible with quantum mechanics must be contextual, i.e. dependent of the measurement arrangement.

The link between non-locality and contextuality as shown by Bell [8] is very close [11, 26]. Proofs of non-locality based on the results of Greenberger, Horne and Zeilinger (GHZ) [22] can be made the basis for a Kochen-Specker theorem [35, 50].

More recently, non-locality and contextuality have been given a unified treatment using algebraic structures from topology [1] and generalizations of Bell inequalities are shown to be violated by contextual and non-local behaviours [2].

We show that every Kochen-Specker set can be used to construct a non-local quantum behaviour that maximally violates a Bell inequality. This is done by using a result by Renner and Wolf [47], which closely links Kochen-Specker sets to pseudo-telepathic games (PT games). We complete the chain by constructing Bell inequalities that are maximally violated by PT games, i.e. the behaviour reaches the algebraic maximum violation for all behaviours.

### 4.2.1 Deriving Bell inequalities

The method we use to derive the Bell inequalities is due to Hardy [24] and has more recently been used and extended in Abramsky and Hardy [2].

Suppose we have propositional formulas $\varphi_1, \ldots, \varphi_N$ and we can assign a probability $p_i$ to each $\varphi_i$.

Now let $P$ be the probability of $\Phi := \bigwedge_i \varphi_i$. We can calculate:

$$\begin{aligned} 1 - P = \mathrm{Prob}(\neg\Phi) &= \mathrm{Prob}(\bigvee_i \neg\varphi_i) \leq \sum_i \mathrm{Prob}(\neg\varphi_i) \\ &= \sum_i (1 - p_i) = N - \sum_i p_i \end{aligned}$$

By rearranging we get $\sum_i p_i \leq N - 1 + P$.

Now if the formulas $\varphi_i$ are jointly contradictory, i.e. $\Phi$ is unsatisfiable, then $P = 0$ and we obtain the inequality

$$\sum_i p_i \leq N - 1. \tag{4.2}$$

In particular we consider formulas where the boolean variables appearing in $\varphi_i$ correspond to empirically testable quantities.

For example, the boolean variables in $\varphi_i$ might be defined for a bipartite behaviour with inputs $a, b \in \{0, \ldots, n-1\}$ and outputs $x, y \in \{0, \ldots, m-1\}$ as

$$\alpha_{x,a} := \begin{cases} \text{true} & \text{if input } a \text{ yields output } x \\ \text{false} & \text{otherwise} \end{cases} \tag{4.3}$$

and

$$\beta_{y,b} := \begin{cases} \text{true} & \text{if input } b \text{ yields output } y \\ \text{false} & \text{otherwise} \end{cases}. \tag{4.4}$$

The probabilistic behaviour rising from such an input-output system is $P(x, y \mid a, b)$, from which the probabilities $p_i$, for certain formulas $\varphi_i$, may be computed.

Observe that for local deterministic behaviours (see Section 3.3.1), the boolean variables are defined by the local deterministic strategies $s, s' \in \{0, \ldots, m-1\}^n$

$$\alpha_{x,a} = \delta_{s_a,x} \quad \beta_{y,b} = \delta_{s'_b,y}$$

with $\delta_{i,j}$ being the Kronecker delta function.

Then, for formulas $\varphi_i, \ldots, \varphi_N$ that are jointly contradictory at least one of the $p_i$ must be zero and any inequality of form (4.2) holds for all local deterministic behaviours. It follows from convexity that any local behaviour satisfies inequalities of form (4.2) and such inequalities are indeed Bell inequalities.

However, there exist probabilistic behaviours and in particular quantum behaviours that violate such inequalities (see Ref. [2] for an illustrated example). This may be explained by the inexistence of a simultaneous global assignment of probabilities to all boolean variables. Making it impossible to assign a probability to $\Phi$, thus invalidating our derivation of the Bell inequality in such a case.

### 4.2.2 Kochen-Specker sets and pseudo-telepathic games

Here we restate the definitions and main results from Ref. [47], while omitting the proofs and detailed constructions.

**Definition 4.1 (Kochen-Specker set)** *A Kochen-Specker set (KS set for short) in $\mathcal{H} = \mathbb{C}^d$ is a set $S \subseteq \mathcal{H}$ of unit vectors such that there exists no function $f : S \to \{0, 1\}$ with the property that if $b \subseteq S$ is an orthonormal basis of $\mathcal{H}$, then*

$$\sum_{u \in b} f(u) = 1$$

*holds.*

**Definition 4.2 (Pseudo-telepathy game)** *Let $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ be a pure state. A pseudo-telepathy game with respect to $|\Psi\rangle$ ($|\Psi\rangle$-PT game for short) is a pair $(B_1, B_2)$, where $B_i$ is a set of orthonormal bases of $\mathcal{H}_i$, such that the following holds. Let $g$ be the function defined on $B_1 \times B_2$ such that $g(b_1, b_2)$ is the set of pairs $(u_1, u_2) \in b_1 \times b_2$ satisfying*

$$\langle\Psi|u_1, u_2\rangle \neq 0.$$

*Then we must have that, for every pair of functions $(s_1, s_2)$, where $s_i$ is defined on $B_i$ and $s_i(b_i) \in b_i$ holds for all $b_i \in B_i$, there must exist particular bases $b_1 \in B_1$ and $b_2 \in B_2$ such that*

$$(s_1(b_1), s_2(b_2)) \notin g(b_1, b_2). \tag{4.5}$$

It follows an abridged version of Theorem 3 from Ref. [47].

**Theorem 4.3 (PT game from KS set)** *Let $S \subseteq \mathcal{H} = \mathbb{C}^d$ be a KS set, then there exists a $|\Psi\rangle$-PT game $(B_1, B_2)$ that can be constructed from $S$. Where*

$$|\Psi\rangle = \frac{1}{\sqrt{n}}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle + \cdots + |d-1\rangle \otimes |d-1\rangle) \in \mathbb{C}^d \otimes \mathbb{C}^d.$$

### 4.2.3 Pseudo-telepathic games and non-locality

We label the inputs and outputs of the behaviour with $x, z$ and $a, c$ to avoid a clash in variables.

**Theorem 4.4 (Non-locality from PT game)** *Let $(B_1, B_2)$ be a PT game with respect to some $|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H}$, then the bipartite quantum $(n, m)$-behaviour*

$$P(x, z \mid a, c) = \mathrm{tr}\left(P_x \otimes P_z |\Psi\rangle\langle\Psi|\right)$$

*with $P_x = |u_x\rangle\langle u_x|$ for $u_x \in b_a \in B_1$ and $P_z = |u_z\rangle\langle u_z|$ for $u_z \in b_c \in B_2$ maximally violates a Bell inequality. Where $n$ is the number of orthonormal basis in $B_1$ and $B_2$ (we assume without loss of generality that the number of basis is equal) and $m = d$, the dimension of the state space $\mathcal{H}$.*

**Proof** First, we construct $N = n^2$ propositional formulas $\varphi_{0,0}, \ldots, \varphi_{n-1,n-1}$ for every possible input pair $a, c$, corresponding to the sets $g(b_a, b_c)$ as defined for PT games.

Let

$$\varphi_{a,c} := \bigvee_{(u_x,u_z)\in g(b_a,b_c)} \left(\alpha_{x,a} \wedge \beta_{z,c} \bigwedge_{(u_{x'},u_{z'})\in(b_a\times b_c)\setminus\{(u_x,u_z)\}} \neg\alpha_{x',a} \wedge \neg\beta_{z',c}\right)$$

with $\alpha_{x,a}$ and $\beta_{z,c}$ as defined in (4.3)–(4.4).

It follows from the definition of PT games that the conjunction of formulas $\varphi_{a,c}$ is unsatisfiable. Assume towards contradiction that there exists an assignment of all $\alpha_{x,a}$ and $\beta_{z,c}$ satisfying the conjunction of the formulas. This assignment can be used to construct a pair of functions $(s_1, s_2)$. Observe that if $\varphi_{a,c}$ is satisfied and $\alpha_{x,a}$ is true then all $\alpha_{x',a}$ for $x' \neq x$ must be false. We can set

$$s_1(a) = u_x \text{ with } \alpha_{x,a} \text{ true}$$

and similarly

$$s_2(c) = u_z \text{ with } \beta_{z,c} \text{ true.}$$

Thus violating (4.5) and leading to contradiction.

Furthermore, we can compute the probabilities $p_{a,c}$ for $\varphi_{a,c}$ from the probabilistic behaviour

$$p_{a,c} = \sum_{(u_x,u_z)\in g(b_a,b_c)} P(x,z \mid a,c) = \sum_{(u_x,u_z)\in g(b_a,b_c)} \langle\Psi|u_x,u_z\rangle^2.$$

Per definition of $g$ we have $p_{a,c} = 1$ for all $a, c$.

We may now use the inequality (4.2)

$$\sum_{a,c} p_{a,c} \leq n^2 - 1.$$

The left hand side evaluates to $n^2$ for the quantum behaviour, which is a violation of this Bell inequality by a value of 1. It follows from the fact that $p_{a,c}$ are probabilities that this is the maximal violation. □

By combining Theorem 4.3 and Theorem 4.4, we have linked every KS set to a quantum behaviour that maximally violates a Bell inequality.

The converse is not entirely clear. While Renner and Wolf showed that a KS set $S \subseteq \mathbb{C}^d$ can be constructed from any $|\Psi\rangle$-PT game (for $|\Psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$ as in Theorem 4.3), it is not evident that every maximal violation of a Bell inequality by a quantum behaviour leads to a PT game. To show this one would need to consider all possible Bell inequalities, which in general (see Ref. [2, Section VI]) are not of form (4.2).

However, one can see that for maximal violations of Bell inequalities of form (4.2) by a quantum behaviour with state $|\Psi\rangle$ as in Theorem 4.3 the sets of measurement basis is a PT game. This follows because for maximal violation the formulas $\varphi_i$ must cover the entire support, corresponding with the function $g$. Being a Bell inequality the formulas must be jointly contradictory, thus ruling out the existence of a pair of function $(s_1, s_2)$ violating (4.5).

This may be seen as an answer to the question raised by Popescu and Rohrlich [45]: "Why does quantum mechanics not violate the CHSH inequality maximally?". The CHSH inequality is of form (4.2) and maximal violation by $|\Psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ would lead to a KS set in $\mathbb{C}^2$, which is not possible [31].

Note that we are not able to retrieve the Tsirelson bound [54] (the quantum mechanical maximal violation) from this argument, only the impossibility of algebraic maximal violation. Also, we are restricted to the case of maximal violation by the maximally entangled state $|\Psi\rangle$ as in Theorem 4.3.

Our argument is slightly stronger in the sense that not only is maximal violation of CHSH impossible by $|\Psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ but also of any chained CHSH inequality [10], which may be expressed in form (4.2) (see Refs. [2, 24]).

Chapter 5

# Computational Methods and Considerations

## 5.1 Deciding Membership in Local Polytope

Pitowksi [40] showed that deciding if a probabilistic behaviour $p$ lies in the interior of the local polytope is NP-complete. Therefore, we do not expect to find an efficient (polynomial time) algorithm. Nevertheless, as the problem may be formulated as a convex optimization, deciding membership in low dimensions is feasible using the following methods and modern computational resources.

### 5.1.1 Finding convex combination

By definition of a polytope (see Section 2.3), if a point $p$ lies in a polytope $\mathcal{P}$, then it may be represented as a convex combination of the extremal points of $\mathcal{P}$. Thus, a point $p$ lies in the local polytope $\mathcal{P}^{\text{local}}$ if and only if it may be represented as a convex combination of the local deterministic behaviours, the extremal points of $\mathcal{P}^{\text{local}}$. Deciding the existence of a convex combination may be formulated as a linear program:

$$\begin{aligned} \text{find } & x_1, \dots, x_s \in \mathbb{R} \\ \text{subject to } & p = \sum_i x_i p_i^{ldb} \\ & \sum_i x_i = 1 \\ & x_i \geq 0 \text{ for all } i = 1, \dots, s. \end{aligned} \tag{5.1}$$

Although this program does not have an objective function it is polynomial equivalent to a general linear program.

As $s$ is exponential in $n$ and $m$ (see Section 3.3.1), deciding if a $(n, m)$-behaviour using this method amounts to solving a linear program with an exponential number of variables and constraints.

### 5.1.2 Separating hyperplane

A standard method in Polyhedral Computation [19] is to consider the following equivalent program. The program (5.1) has a solution if and only if the following has no solution:

$$\begin{aligned} \text{find } & z \in \mathbb{R}^d, z_0 \in \mathbb{R} \\ \text{subject to } & z^\top p_i^{ldb} - z_0 \leq 0 \text{ for all } i = 1, \dots, s \\ & z^\top p - z_0 > 0. \end{aligned} \tag{5.2}$$

Which amounts to fitting a separating hyperplane $(z, z0)$ between the polytope (its extremal points) and the point $p$. If such a hyperplane exists, then $p$ does not lie in the polytope. This may also be shown directly from the separating and supporting hyperplane theorem [9, p. 46ff.].

Note that this corresponds to the the dual program of (5.1).

In practice we will use following linear program:

$$\begin{aligned} \text{maximize } & z^\top p - z_0 \\ \text{subject to } & z^\top p_i^{ldb} - z_0 \leq 0 \text{ for all } i = 1, \dots, s \\ & z^\top p - z_0 \leq 1. \end{aligned} \tag{5.3}$$

The last inequality is added to prevent arbitrary scaling of the hyperplane, which would lead to an unbounded solution.

If the objective value of the linear program (5.3) is greater than zero $z^\top p - z_0 > 0$, then $(z, z0)$ is a solution to the program (5.2) and thus $p$ does not lie in the local polytope.

We are able to make a minor improvement by assuming that the point $p$ lies in the non-signaling vector subspace. The following proposition follows directly from the proof of the supporting hyperplane theorem. Nevertheless, we give an explicit proof.

**Proposition 5.1** *For every non-signaling,non-local point $p \in \mathcal{V}^{ns} \setminus \mathcal{P}^{local}$, there exists a supporting hyperplane $(z, z_0)$ with $z \in \mathcal{V}^{ns}$ and some $r \in \mathcal{P}^{local}$ satisfying*

$$z^\top u - z_0 \leq 0 \text{ for all } u \in \mathcal{P}^{local}, \tag{5.4}$$

$$z^\top r - z_0 = 0 \tag{5.5}$$

*and*

$$z^\top p - z_0 > 0. \tag{5.6}$$

**Proof** By proposition 2.5, there exists a unique point $r \in \mathcal{P}^{\text{local}}$ with minimal distance to $p$

$$\|p - r\| = \min\left\{\|p - r'\| \mid r' \in \mathcal{P}\right\}. \tag{5.7}$$

Let $z = (p - r)$ and $z_0 = (p - r)^\top r$. We have $z \in \mathcal{V}^{\text{ns}}$. Conditions (5.6) and (5.5) follow

$$z^\top p - z_0 = (p - r)^\top (p - r) = \|p - r\|^2 > 0$$

and

$$z^\top r - z_0 = (p - r)^\top (r - r) = 0.$$

To show the remaining conditions, assume towards contradiction there exists a point $u \in \mathcal{P}^{\text{local}}$ with

$$z^\top u - z_0 = (p - r)^\top (u - r) > 0. \tag{5.8}$$

Consider the point $(1 - c)r + cu = r + c(u - r) \in \mathcal{P}^{\text{local}}$ with $0 \leq c \leq 1$ (membership in $\mathcal{P}^{\text{local}}$ follows from convexity of the polytope). We have for the derivative of the squared distance to $p$ evaluated at $c = 0$:

$$\frac{d}{dc} \|p - (r + c(u - r))\|^2 \bigg|_{c=0} = 2(r - p)^\top (u - r).$$

By (5.8) the term above is negative. Thus, we are able to find a point $r + c(u - r)$ for some $c$ with smaller distance to $p$. This in contradiction with (5.7), concluding the proof. $\square$

Using proposition 5.1 we see that if $p \in \mathcal{V}^{\text{ns}}$ it suffices to find a hyperplane $(z, z_0)$ with $z \in \mathcal{V}^{\text{ns}}$.

$$\begin{aligned} &\text{maximize } z^\top p - z_0 \text{ with } z \in \mathcal{V}^{\text{ns}} \\ &\text{subject to } z^\top p_i^{ldb} - z_0 \leq 0 \text{ for all } i = 1, \ldots, s \\ &\qquad\qquad z^\top p - z_0 \leq 1. \end{aligned} \tag{5.9}$$

Note that we do not need to specify the non-signaling constraints in the linear program directly but instead use a basis of the non-signaling pace $B^{\text{ns}}$ (see Section 3.2) and optimize over a variable $x$ so that $z = B^{\text{ns}} x$.

## 5.2 Distance From Boundary of Local Polytope

Given a point $p \in \mathcal{P}^{\text{local}}$ one may be interested in how close this behaviour is to the boundary of the local polytope $\mathcal{P}^{\text{local}}$.

In our context, we are more precisely interested in the distance to the closest non-local behaviour, i.e. to the non-trivial border of the polytope. We need to make this distinction as the local polytope is defined by boundaries shared by all probabilistic behaviours (trivial Bell inequalities) and boundaries to non-local,non-signaling behaviours (non-trivial Bell inequalities).

In the following we discuss a few methods to compute the distance to the non-trivial boundary of the local polytope and find non-signaling and non-local behaviours close to some local behaviour $p$.

### 5.2.1 Convex hull

One possible approach would be to compute the convex hull of the local polytope, that is compute the halfspace representation of $\mathcal{P}^{\text{local}}$, verifying non-triviality of the Bell inequalities (see Section 5.3.1) and compute the minimal distance.

However, computing the halfspace representation (known as the convex hull problem) is in general not easy [19], especially considering that the number of local deterministic behaviours defining the polytope $\mathcal{P}^{\text{local}}$ is exponential in $n$ (see Section 3.3.1). In our case this method is not feasible.

### 5.2.2 Rays to non-local boxes

The distance from a point $p \in \mathcal{P}^{\text{local}}$ to a non-trivial boundary may also be computed by considering the *non-local boxes* (also called Popescu-Rohrlich boxes), the non-local extremal vertices of the non-signaling polytope $\mathcal{P}^{\text{ns}}$.

A non-local box $p' \in \mathcal{P}^{\text{ns}}$ lies outside the local polytope $\mathcal{P}^{\text{local}}$, i.e. there exists a non-trivial boundary between $p$ and $p'$. By placing a ray from $p$ to $p'$ and using bisection one may find a point $cp + (1-c)p' \in \mathcal{P}^{\text{local}}$ on the boundary of the local polytope. If this can be done systematically for all non-local boxes, then the distance from point $p$ to the non-trivial boundary of $\mathcal{P}^{\text{local}}$ may be computed.

Jones and Masanes [30] have given a complete characterization of all the non-local boxes for arbitrary number of inputs $n$ and $m = 2$. However, the number of non-local boxes is extremely large even for small $n$, making a systematic approach infeasible.

### 5.2.3 Sampling

If a point $p \in \mathcal{P}^{\text{local}}$ is close to a non-trivial boundary, then by sampling in a region around $p$ we hope to find non-signaling and non-local points $p' \in \mathcal{P}^{\text{ns}} \setminus \mathcal{P}^{\text{local}}$ close to $p$.

In particular we consider the affine space of normalized non-signaling points $\mathcal{A}^{\text{ns-norm}} \subsetneq \mathcal{V}^{\text{ns}}$, the space of points in $\mathcal{V}^{\text{ns}}$ satisfying the normalization conditions. This space is defined by a finite number of linear equalities

$$C^{\text{ns-norm}} q = (0, \dots, 0, 1, \dots, 1)^\top$$

which consists of the equalities $C^{\text{ns}}$, imposing the non-signaling condition (see Section 3.2), and the non-homogeneous equalities ensuring the normalization condition (see Section 3.1).

Using the relationship between the solution space of homogeneous and non-homogeneous systems of linear equations, as described in Section 2.1.2, we can find an orthonormal basis $B^{\text{ns-norm}}$ such that

$$\mathcal{A}^{\text{ns-norm}} = \{p + B^{\text{ns-norm}} x | x \in \mathbb{R}^d\}$$

where $d$ is the dimension of $\mathcal{A}^{\text{ns-norm}}$. Note that $p \in \mathcal{P}^{\text{local}} \subsetneq \mathcal{A}^{\text{ns-norm}}$.

By choosing random $x$ such that $\|x\| = \varepsilon$ we are able to sample points $p' \in \mathcal{A}^{\text{ns-norm}}$ lying on an $\varepsilon$-sphere around $p$. Note, however, that $p'$ obtained by such sampling is not necessarily a non-signaling behaviour $p' \in \mathcal{P}^{\text{ns}}$, it may not satisfy the non-negativity condition (see Section 3.1).

In order to find $p' \in \mathcal{P}^{\text{ns}} \setminus \mathcal{P}^{\text{local}}$ we use following procedure, given $B^{\text{ns-norm}}$ and some $\varepsilon$:

1. Choose $x \in \mathbb{R}^d$ randomly with $\|x\| = \varepsilon$ and set $p' = p + B^{\text{ns-norm}} x$.
2. If $p'_{x,y,a,b} \geq 0$ for all $x, y, a, b$ ($p' \in \mathcal{P}^{\text{ns}}$), then continue. If $p'$ does not satisfy non-negativity condition ($p' \notin \mathcal{P}^{\text{ns}}$), then reject $p'$.
3. Decide if $p' \in \mathcal{P}^{\text{local}}$ (see Section 5.1). If $p' \notin \mathcal{P}^{\text{local}}$, then output $p' \in \mathcal{P}^{\text{ns}} \setminus \mathcal{P}^{\text{local}}$.

If the procedure outputs a $p' \in \mathcal{P}^{\text{ns}} \setminus \mathcal{P}^{\text{local}}$ for some $\varepsilon$, then $\varepsilon$ is an upper bound of the distance between $p$ and the non-trivial border of $\mathcal{P}^{\text{local}}$.

Note, however, that the rejection rate in step 2 can be very high.

For large $\varepsilon$ (close to the diameter of the local polytope) many sampled points will lie outside of the non-signaling polytope $\mathcal{P}^{\text{ns}}$, as its diameter coincides with the diameter of the local polytope (see Proposition 3.6). Thus, this method, in general, is unsuitable for estimating the distance to the non-trivial border by variation of $\varepsilon$.

Also, if $p$ contains elements with value zero, then it lies on a non-trivial border shared by the non-signaling polytope and many sampled points, even with small $\varepsilon$, will be rejected.

On the other hand, if we do find a point $p' \in \mathcal{P}^{\text{ns}} \setminus \mathcal{P}^{\text{local}}$ for very small $\varepsilon$ (large enough to be able to use computational methods), then we have good indication that $p$ lies on a non-trivial Bell inequality, or at least very close to one. Given such a point $p'$ we can find a Bell inequality, which may be interesting for further study (see Section 5.3).

Furthermore, if $p \in \mathcal{P}^{\text{local}}$ does in fact lie on a non-trivial Bell inequality, then with high probability (at least $\frac{1}{2}$) the sampled points $p' \in \mathcal{P}^{\text{ns}}$ will be non-local. This is because the non-trivial Bell inequality is a hyperplane separating the space, we sample from, into two halfspaces. If we randomly sample $p' \in \mathcal{P}^{\text{ns}}$ we will with high probability get a non-local point $p'$. The rejection rate, however, may be very high.

#### Zero constraints

If we have a point $p \in \mathcal{P}^{\text{local}}$ containing elements with value zero we may consider an alternate space from which to sample point from.

Let $C^{\text{ns-norm-zero}}$ be a system of linear equations with equations corresponding to $C^{\text{ns-norm}}$ and additional constraints for every element $p_i = 0$ fixing the value of the element at position $i$ to zero. Consider the resulting affine space $\mathcal{A}^{\text{ns-norm-zero}}$ and corresponding orthonormal basis $B^{\text{ns-norm-zero}}$.

We have for every element at position $i$ with $p_i = 0$

$$p'_i = 0 \text{ for all } p' \in \mathcal{A}^{\text{ns-norm-zero}}.$$

Using the procedure as described above, we can find $p' \in \mathcal{P}^{\text{ns}} \cap \mathcal{A}^{\text{ns-norm-zero}}$.

By including the zero constraints we decrease the chance of sampling a point $p' \notin \mathcal{P}^{\text{ns}}$, as the elements with value zero, which are most likely to result in a negative point, remain zero.

We use the procedure on this zero-constrained space with small $\varepsilon$ to decide if some behaviour $p \in \mathcal{P}^{\text{local}}$ lies on a non-trivial Bell inequality.

Finding a point $p' \in (\mathcal{P}^{\text{ns}} \cap \mathcal{A}^{\text{ns-norm-zero}}) \setminus \mathcal{P}^{\text{local}}$ close to some $p \in \mathcal{P}^{\text{local}}$, implies that $p$ is on or close to a non-trivial Bell inequality. The converse, however, does not hold. There could exist a non-trivial Bell inequality $(z, z_0)$ with $z$ in the orthogonal complement of the sample space. The separating hyperspace defined by $(z, z_0)$ would lie on (or parallel to) the sample space and any sampled point would lie on (or parallel to) the non-trivial Bell inequality.

## 5.3 Finding Bell Inequalities

If $p'$ is a non-signaling and non-local behavior, then placing a separating hyperplane between $p'$ and the local polytope (see Section 5.1.2) results in a non-trivial Bell inequality. By using the methods described in Section 5.2.2 and 5.2.3 we may find such a behaviour $p'$ close to some behavior $p \in \mathcal{P}^{\text{local}}$.

We use these methods, in particular the sampling procedure, to find non-local, non-signaling behaviours $p'$ and non-trivial Bell inequality. The hope is that this results in Bell inequalities that are in some sense close to a local behaviour of interest $p \in \mathcal{P}^{\text{local}}$.

### 5.3.1 Trivial or non-trivial Bell inequality

In some situations it is not entirely clear if a Bell inequality is trivial or not. We use following method to check non-triviality of a Bell inequality.

Deciding if a Bell inequality is trivial or not can be done by maximizing the violation of the inequality over all non-signaling behaviours. If there exists a non-signaling behavior that violates the inequality, the Bell inequality is non-trivial.

Given a Bell inequality $(z, z_0)$, we use the following linear program

$$\begin{aligned} \text{maximize } & z^\top p - z_0 \text{ with } p \in \mathcal{V}^{\text{ns}} \\ \text{subject to } & \sum_{x,y} p_{x,y,a,b} = 1 \text{ for all } a, b \\ & p_{x,y,a,b} \geq 0 \text{ for all } x, y, a, b. \end{aligned} \tag{5.10}$$

The constraints impose the the normalization and non-zero condition of behaviours (see Section 3.1).

If the objective value $z^\top p - z_0 > 0$ then $p$ is a non-signaling behavior and $(z, z_0)$ a non-trivial Bell inequality.

## 5.4 Implementation

The methods mentioned above have been implemented using MATLAB, the convex optimization toolbox `CVX` and the quantum information toolbox `QLib` [33]. The implementation is available online[1].

[1] `http://cqi.inf.usi.ch/publications.html`

Chapter 6

# Three-Partite Marginal Quantum Non-Locality

As mentioned in Section 4.1, it is not clear which entangled states admit non-local behaviour. Here we investigate the bipartite reduced states of three-partite states for non-local behaviour.

## 6.1 Setting

We are interested in finding a three-partite quantum state $\rho_{ABC} \in \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C)$, such that the three bipartite reduced states

$$\rho_{AB} = \mathrm{tr}_C(\rho_{ABC}) \quad \rho_{AC} = \mathrm{tr}_B(\rho_{ABC}) \quad \rho_{BC} = \mathrm{tr}_A(\rho_{ABC})$$

admit non-local behaviour

$$\mathcal{C}^{\mathrm{Q}}_{\rho_{AB}} \nsubseteq \mathcal{P}^{\mathrm{local}} \quad \mathcal{C}^{\mathrm{Q}}_{\rho_{AC}} \nsubseteq \mathcal{P}^{\mathrm{local}} \quad \mathcal{C}^{\mathrm{Q}}_{\rho_{BC}} \nsubseteq \mathcal{P}^{\mathrm{local}}. \tag{6.1}$$

Given such a state we can construct a quantum behaviour for $\rho_{ABC}$

$$P(x, y, z \mid a, b, c)$$

such that the marginals $P(x, y \mid a, b), P(x, z \mid a, c)$ and $P(y, z \mid b, c)$ are non-local quantum behaviours for the respective reduced states. Thus explaining the term *three-partite marginal quantum non-locality*.

#### Trivial example

Consider the following pure state with the singlet $|\Phi\rangle = \frac{1}{\sqrt{2}}|00\rangle + |11\rangle$

$$|\psi\rangle = |\Phi\rangle_{12} \otimes |\Phi\rangle_{34} \otimes |\Phi\rangle_{56} \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \mathcal{H}_4 \otimes \mathcal{H}_5 \otimes \mathcal{H}_6.$$

If $\mathcal{H}_A = \mathcal{H}_1 \otimes \mathcal{H}_3$, $\mathcal{H}_B = \mathcal{H}_2 \otimes \mathcal{H}_5$ and $\mathcal{H}_C = \mathcal{H}_4 \otimes \mathcal{H}_6$, then clearly $\rho_{ABC} = |\psi\rangle\langle\psi|$ satisfies (6.1).

Observe that the marginal non-local behaviours $P(x, y \mid a, b)$ and $P(y, z \mid b, c)$, fully defined by $\rho_{AB} = |\Phi\rangle\langle\Phi|_{12} \otimes I_3 \otimes I_5$ and $\rho_{BC} = I_2 \otimes I_4 \otimes |\Phi\rangle\langle\Phi|_{56}$ respectively, do not imply non-locality of $P(x, z \mid a, c)$ only assuming non-signaling of $P(x, y, z \mid a, b, c)$.

As shown by Coretti, Hänggi and Wolf [13], finding a quantum state admitting non-local behavior satisfying such a transitivity property might be valuable in ruling out certain alternative models for the explanation of quantum correlations. Moreover, such a state is interesting in itself, shedding light on the character of quantum non-locality.

In the following we will study states that are likely to admit such behaviours.

## 6.2 The W-State

The W-state is a three-partite qubit state defined by

$$|W\rangle = \frac{1}{\sqrt{3}} \left(|001\rangle + |010\rangle + |100\rangle\right) \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C.$$

We have for $\rho_{ABC} = |W\rangle\langle W|$ the bipartite reduced states

$$\rho_{AB} = \rho_{AC} = \rho_{BC} = \frac{1}{3}|00\rangle\langle 00| + \frac{2}{3}|\Psi^+\rangle\langle\Psi^+|$$

with $|\Psi^+\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle + |10\rangle\right)$.

Because of the equivalence of the bipartite reduced states, showing that the reduced state $\rho_{AB}$ admits non-local behaviour $\mathcal{C}^{Q}_{\rho_{AB}} \not\subseteq \mathcal{P}^{\text{local}}$ implies that all bipartite reduced states admit non-local behaviour, the state satisfies (6.1).

We have that the bipartite reduced states are entangled. Furthermore, Dür et al. [14] showed that of all three-partite qubits the bipartite reduced states of the W-state are maximally entangled.

In a recent result, Sawicki et al. [48] showed that the W-state is determined by its single party reduced states and thus also by the bipartite reduced states $\rho_{AB}$ and $\rho_{BC}$. We have the property that given $\rho_{AB}$ and $\rho_{BC}$, $\rho_{AC}$ is fully determined. Even tough this alone does not imply the transitivity property for non-local behaviours, as described above, it seems like a positive step towards showing such a property.

### 6.2.1 Monogamy

If a pure bipartite quantum state is entangled, then it is not entangled with any other system. This is called the *monogamy of entanglement*.

For mixed states this is not the case. As seen above, an entangled mixed bipartite state can be entangled to a third system. On a lighter note, such states, e.g. the W-state, are sometimes said to be promiscuous.

Consider the following symmetric case. Let $\rho_{AB}$ be any bipartite quantum state. We call $\rho_{AB}$ $N$-shareable if there exists a $(N+1)$-partite state $\rho_{AB_1B_2\cdots B_N}$ so that $\rho_{AB} = \rho_{AB_i}$ for all $i$.

We have that a bipartite quantum state is $N$-shareable for all $N$ (also called $\infty$-shareable) if and only if it is separable (not entangled) [49].

One can easily see that the bipartite reduced states of the W-state are at most 2-shareable, the symmetric extension being the W-state.

Regarding behaviours we have another result by Terhal et al. [52]. If a bipartite quantum state $\rho_{AB}$ is $N$-shareable then any quantum behaviour with $N$ or less measurement settings per party does not violate any Bell inequality. In other words, any quantum $(n, m)$-behavior for $\rho_{AB}$ with $n \leq N$ is local.

This may be seen as a complement to a result by Masanes et al. [34], who proved that any $N$-shareable non-signaling behaviour is local for $N$ measurement settings.

For the reduced states of the W-state this means that we can not expect to violate a Bell inequality for $n = 2$. Non-local behaviours, in general, are not ruled out by this result.

Note, that the W-state expresses more symmetry than required for the Terhal result. While Terhal only requires for a symmetric extension $\rho_{AB_1B_2}$ so that $\rho_{AB} = \rho_{AB_1} = \rho_{AB_2}$, for the W-state we additionally have $\rho_{AB} = \rho_{B_1B_2}$. Wether this condition implies stronger monogamy constraints is not known (or the author is unaware of any such results). Finding non-local behaviour on the bipartite reduced state of such a highly symmetric state would be interesting in respect to such considerations.

### 6.2.2 Quest for non-locality

Having motivated the interest for such non-locality of the W-state we used tools presented in Chapter 5 towards finding such non-locality. However, no non-local behavior for the bipartite reduced state of the W-state was found and neither were we able to construct a local hidden variable model (as Werner did for Werner states). Nevertheless, we find indications that the bipartite states does not admit non-local behaviour.

#### Measurement in standard basis

We know that the quantum behaviour achieved by measuring $|\Psi^+\rangle$ in standard bases lies on a non-trivial face, i.e. non-trivial Bell inequality, of the local polytope $\mathcal{P}^{\text{local}}$, while slightly rotating the bases results in non-local behaviour.

On the other hand, measuring $|00\rangle$ in standard bases results in perfect correlation, whereas slight rotations only increases non-correlated noise. Measuring in the diagonal basis only results in noise, i.e. the outcomes $(0,0)$, $(0,1)$, $(1,0)$ and $(1,1)$ are equally likely.

For the bipartite reduced state $\rho_{AB}$, which can be expressed as mixture of $|00\rangle$ and $|\Psi^+\rangle$, we expect to see, if at all, non-local behaviour while slightly rotating the measurement bases from the standard basis. As large angles of rotation result in high amount of non-correlated noise. We expect, if the state admits non-local behaviour, that the behaviour for measurement in standard bases lies on a non-trivial face of the local polytope $\mathcal{P}^{\text{local}}$ for some $n$.

Let $P^{\text{sb}}(x,y \mid a,b)$ be the quantum $(n,2)$-behaviour achieved by measuring the bipartite reduced state $\rho_{AB}$ in the standard basis for all $n$ measurement settings. We have for all $a,b$

$$
\begin{aligned}
P^{\text{sb}}(0,0 \mid a,b) &= \operatorname{tr}\left(|0\rangle\langle 0| \otimes |0\rangle\langle 0| \rho_{AB}\right) = 1/3, \\
P^{\text{sb}}(1,0 \mid a,b) &= \operatorname{tr}\left(|1\rangle\langle 1| \otimes |0\rangle\langle 0| \rho_{AB}\right) = 1/3, \\
P^{\text{sb}}(0,1 \mid a,b) &= \operatorname{tr}\left(|0\rangle\langle 0| \otimes |1\rangle\langle 1| \rho_{AB}\right) = 1/3 \text{ and} \\
P^{\text{sb}}(1,1 \mid a,b) &= \operatorname{tr}\left(|1\rangle\langle 1| \otimes |1\rangle\langle 1| \rho_{AB}\right) = 0.
\end{aligned}
$$

In matrix notation (see Section 3.1) the behaviour has following form

$$
\begin{pmatrix}
1/3 & 1/3 & \cdots \\
1/3 & 0 & \cdots \\
\vdots & \vdots & \ddots
\end{pmatrix}
$$

with the top left block repeated $n^2$ times. We will call the corresponding vector, as in (3.1), $p^{\text{sb}} \in \mathbb{R}^{n^k \cdot m^k}$.

#### Trivial Bell inequality

Note that $p^{\text{sb}}$ in fact lies on the border of the local polytope $\mathcal{P}^{\text{local}}$, i.e. it lies on a Bell inequality.

Consider the inequality $(z, z_0)$ (in matrix form) with following blocks

$$
\begin{pmatrix}
0 & 0 \\
0 & -1
\end{pmatrix}.
$$

and $z_0 = 0$. We have $z^\top p^{\text{sb}} - z_0 = 0$ and $z^\top p - z_0 \leq 0$ for all $p$ non-negative and in particular all $p \in \mathcal{P}^{\text{ns}}$, it is a trivial Bell inequality (see Section 3.3.2).

Whether $p^{\text{sb}}$ also lies on a non-trivial Bell inequality can not be ruled out by this argument. However, we find indications that the point does not lie on such a Bell inequality.

### Non-trivial Bell inequality

Here we present indications that $p^{\text{sb}}$ does not lie on a non-trivial Bell inequality.

First, observe that $p^{\text{sb}}$ lies in a polytope defined by exponentially many local deterministic behaviours.

**Proposition 6.1** *The point $p^{sb}$ lies in the interior of a polytope defined by $2^{n+1}-1$ local deterministic behaviours as extremal points.*

**Proof** We proceed by defining the set of local deterministic behaviours defining the polytope and show a convex combination of $p^{\text{sb}}$ with all coefficients non-zero. From the existence of such a convex combination it follows that the point does not lie in the interior of the polytope.

Observe that $p^{\text{sb}}$ is zero at elements with output $x=1$ and $y=1$ for all inputs $a,b$. That is, $p^{\text{sb}}$ can not be expressed as convex combination with non-zero coefficient for local deterministic behaviours that output $x=1$ and $y=1$ for any $a,b$. Let $\mathcal{P}'$ be the polytope defined by all local deterministic behavior that do not output $x=1$ and $y=1$.

Consider the local deterministic strategy (see Definition 3.3) $s,s'$ for the behaviours defining $\mathcal{P}'$. If an element $s_a=1$ then we have that $s'=(0,\ldots,0)$ as otherwise the local deterministic behaviour would output $(1,1)$ for input $a$ and some $b$. We can now count the number of such deterministic behaviours/strategies. All $2^n$ possible string $s\in\{0,1\}^n$ are possible when $s'=(0,\ldots,0)$ and vice versa, thus we have $2\cdot 2^n$ pairs of strategies. Note that we count the strategy $s=(0,\ldots,0)$ and $s'=(0,\ldots,0)$ twice, thus the total number of strategies and local deterministic behaviours defining the polytope is $2^{n+1}-1$.

Now to construct the convex combination. Consider the case where $s\in\{0,1\}^n$ and $s'=(0,\ldots,0)$. Let $\bar{s}\in\{0,1\}^n$ be the string with $s_a=1\Leftrightarrow\bar{s}_a=0$ for all $a$. Then the combination (not convex) $\frac{1}{3}p^{\text{ldb}}_{s,s'}+\frac{1}{3}p^{\text{ldb}}_{\bar{s},s'}$ is, in matrix form, a matrix with following blocks

$$\begin{pmatrix}1/3 & 0\\ 1/3 & 0\end{pmatrix}.$$

By adding another local deterministic behaviour with $r=(0,\ldots,0)$ and $r'=(1,\ldots,1)$ we get the convex combination $\frac{1}{3}p^{\text{ldb}}_{s,s'}+\frac{1}{3}p^{\text{ldb}}_{\bar{s},s'}+\frac{1}{3}p^{\text{ldb}}_{r,r'}=p^{\text{sb}}$. The case where $s=(0,\ldots,0)$ and $s'\in\{0,1\}^n$ is symmetric.

We have shown that $p^{\mathrm{sb}}$ can be expressed as convex combination including any local deterministic behaviour defining the polytope. All these convex combinations can be used to construct a convex combination including all extremal points with non-negative coefficients (a convex combination of a convex combination). It follows straightforwardly that $p^{\mathrm{sb}}$ can not lie on the border of the polytope $\mathcal{P}'$, concluding the proof. □

From Proposition 6.1 follows a condition for (non-trivial) Bell inequalities on which $p^{\mathrm{sb}}$ lies.

**Proposition 6.2** *If $p^{sb}$ lies on a Bell inequality, then so do exponentially many local deterministic behaviours.*

**Proof** Let $(z, z_0)$ be a Bell inequality with

$$z^\top p^{\mathrm{sb}} - z_0 = 0.$$

From Proposition 6.1 it follows that there exists a convex combination of $p^{\mathrm{sb}}$ with $N = 2^{n+1} - 1$ local deterministic behaviours $p_i^{\mathrm{ldb}} \in \mathcal{P}^{\mathrm{local}}$

$$p^{\mathrm{sb}} = \sum_i^N c_i p_i^{\mathrm{ldb}}$$

with $c_i > 0$ for all $i$.

We have

$$z^\top \left( \sum_i^N c_i p_i^{\mathrm{ldb}} \right) - z_0 = 0.$$

Using $z_0 = \sum_i^N c_i z_0$, we get

$$\sum_i^N c_i z^\top p_i^{\mathrm{ldb}} - c_i z_0 = 0. \tag{6.2}$$

Note that $(c_i z, c_i z_0)$ is simply a scaling of the hyperplane $(z, z0)$ (see Section 2.1.3) and as $p_i^{\mathrm{ldb}} \in \mathcal{P}^{\mathrm{local}}$

$$c_i z^\top p_i^{\mathrm{ldb}} - c_i z_0 \leq 0$$

for all $i$. It follows from (6.2) that $c_i z^\top p_i^{\mathrm{ldb}} - c_i z_0 = 0$ and in particular

$$z^\top p_i^{\mathrm{ldb}} - z_0 = 0$$

for all $i$. That is, all $2^{n+1} - 1$ local deterministic behaviours $p_i^{\mathrm{ldb}}$ lie on the Bell inequality $(z, z0)$, concluding the proof. □

As can be easily verified, the trivial Bell inequality, as presented in the section above, satisfies Proposition 6.2.

Furthermore, we observe that the local deterministic behaviours defined by $s = s' = (0, \ldots, 0)$ is in the polytope $\mathcal{P}'$ from Proposition 6.1 and lies on a non-trivial Bell inequality, a chained CHSH inequality. While the local deterministic behaviour defined by $s = (1, \ldots, 1)$ and $s' = (0, \ldots, 0)$, also in $\mathcal{P}'$, lies on a distinct variant of the chained CHSH inequality.

In conclusion, if there exists a non-trivial Bell inequality $(z, z_0)$ that $p^{\text{sb}}$ lies on, then so do exponentially many local deterministic behaviours and some of these local deterministic behaviours lie on at least two distinct non-trivial Bell inequalities. While we were not able to find a geometric argument ruling out the possibility of such non-trivial Bell inequalities, the existence of such inequalities seems unlikely.

Computational methods, as described in Chapter 5, were used in order to find such a non-trivial Bell inequality. However, we were not able to find a non-trivial Bell inequality for $n \leq 5$ using the sampling method (see Section 5.2.3). For higher dimensions, the rejection rate is too large.

We observe, computationally, that for $n \leq 14$ the zero-constrained space $\mathcal{P}^{\text{ns}} \cap \mathcal{A}^{\text{ns-norm-zero}}$ coincides with the reduced polytope $\mathcal{P}'$ from Proposition 6.1, thus finding a Bell inequality on which $p^{\text{sb}}$ lies by sampling in the zero-constrained space does not work in this case.

Even tough we can not formally rule out non-local behaviour, our findings indicate that the bipartite reduced states of the W-state do not admit non-local behaviour.

## 6.3 Beyond Qubits

As we have indications that the W-state and thus possibly all three-partite qubit states do not admit non-local behaviour for all bipartite reduced states, we investigate three-partite states of higher dimension.

Consider the three-partite qutrit Aharonov state [17]:

$$|A\rangle = \frac{1}{\sqrt{6}} \left( |012\rangle + |120\rangle + |201\rangle - |021\rangle - |102\rangle - |210\rangle \right).$$

We have for $\rho_{ABC} = |A\rangle\langle A|$ the bipartite reduced states

$$\rho_{AB} = \rho_{AC} = \rho_{BC} = \frac{1}{3}|\Psi_{01}^-\rangle\langle\Psi_{01}^-| + \frac{1}{3}|\Psi_{02}^-\rangle\langle\Psi_{02}^-| + \frac{1}{3}|\Psi_{12}^-\rangle\langle\Psi_{12}^-|$$

with $|\Psi_{ij}^-\rangle = \frac{1}{\sqrt{2}} \left( |ij\rangle - |ji\rangle \right)$.

Observe that $\rho_{AB}$ is in fact a Werner state for $d = 3$ and $\alpha = 1$ and as $\alpha > 1/4$ the reduced state is entangled (see Section 4.1.1).

Despite the prominence of this state, the author was unable to find any results indicating whether it admits non-local behaviour.

Nevertheless, Werner's local model is only for the state with $\alpha = 2/3$

$$\frac{2}{3}\rho_{AB} + \frac{1}{27}I.$$

Thus, non-local behaviour is not impossible due to the results by Werner.

Again using the quantum behaviour for measurements in standard basis ($m = 3$) as starting point $p^{\text{sb}}$ we apply the sampling method, as described in Section 5.2.3, to find interesting non-trivial Bell inequalities. The point $p^{\text{sb}}$ does not seem to lie on a non-trivial Bell inequality for $n \leq 4$. Using the zero constrained method, we were unable to find a non-trivial Bell inequality for $n \leq 5$.

For higher dimensions, simply computing the local deterministic behaviours and deciding membership in the local polytope is very inefficient as there are $3^{2n}$ such behaviours (see Section 3.3.1).

Also, no non-local behaviour was found using measurements with rotated bases (various rotations around various rotation axes).

Chapter 7

# Discussion

*"Begin at the beginning," the King said gravely, "and go on till you come to the end: then stop."*

— Lewis Carroll, *Alice in Wonderland*

Even tough we were not able to find three-partite marginal quantum non-locality, we have found indications that no three-partite qubit state, in particular the W-state, admits such behaviour. As the computational methods reach their limits, we propose an analytical inquiry for a local model and a study of the monogamy constraints that may be implied by the symmetries of the W and similar states.

We investigated the Aharonov state, a three-partite qutrit state with symmetric and entangled bipartite reduced states, but were not able to find non-local behaviour for the bipartite states. However, further inquiry is well justified given not only the possibility of three-partite marginal non-locality but also the bipartite reduced states relationship to the results of Werner. This relationship might be used for a more analytical study which is more robust to the high dimensions than the computational methods we used.

Nevertheless, the computational methods presented, discussed and implemented in Chapter 5 might be useful for future experiments and studies including probabilistic behaviours.

In Chapter 4 we have shown that a bipartite non-local quantum behaviour that maximally violates a Bell inequality can be constructed from any Kochen-Specker set. This not only sheds light on to the relationship between contextuality and non-locality but also is an example of bipartite non-local quantum behaviour that reaches the maximal algebraic violation of a Bell inequality. Whereas multipartite maximally non-local quantum behaviour has been known to exist in the form of GHZ type non-locality [2], the author is unaware of previous results showing maximally non-local bipartite quantum behaviours.

As mentioned, the converse, that every maximally non-local bipartite quantum behaviour leads to a Kochen-Specker set, holds for a certain class of Bell inequality and a maximally entangled state. As there are no Kochen-Specker sets in two dimensional space, this may be seen as an answer to the question raised by Popescu and Rohrlich [45], why Quantum Mechanics does not maximally violate the CHSH inequality. A generalization to a greater class of Bell inequalities and states might provide valuable insight to the relationship between contextuality and non-locality as well as to the question of which states admit non-local behaviour.

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