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Exploring the Interplay between Entanglement and Nonlocality

A Novel Perspective on the Peres Conjecture

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Untersuchungen des Zusammenspiels von Verschränkung und Nichtlokalität

Ein neuer Blick auf die Peres-Vermutung

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1. Introduction

One of the most intriguing features of quantum mechanics is entanglement. Entangled systems can display correlations that go beyond our classical intuition. Nevertheless, these correlations have been observed and confirmed by a great number of experiments.¹ In addition, entanglement is a resource for quantum information processing tasks that have no classical analogue. It can be used to encrypt messages securely via quantum key distribution [BBB⁺92] or to transmit a quantum state over arbitrary distances [BPM⁺97]. Intensive studies of entanglement have also led to new insights on the structure of low energy states of physical systems [Oru14].

A fascinating aspect of entanglement is that the correlations between entangled particles do not always admit a local hidden variable (LHV) model.² In other words, entanglement sometimes implies nonlocality. The precise connection between these two concepts, however, is not known to date. While we know that entanglement is necessary to obtain nonlocal effects, there are entangled states that admit an LHV model. Over the past few decades various attempts have been made to limit the number of possible states implying nonlocality. In this thesis we will focus on one particular conjecture by Asher Peres [Per98]. He suggested that a certain set of states, so-called PPT states, admits a description via local models. His conjecture was disproved years later, when Vertési and Brunner found a PPT-state that does not admit an LHV model [VB12, VB14]. A counterexample does not provide much insight into the connection between PPT-states and locality, though. The aim of this thesis is to study the Peres conjecture more closely for a particular scenario. To do so, we first recapitulate the necessary theoretical foundations. Then we introduce a novel method that allows us to obtain new results numerically while providing an analytical proof for these results on the side.

The work is structured as follows. In Chapter 2 we will review the postulates of quantum mechanics, which lay the foundations for the following discussion. In Chapter 3 we will discuss entanglement and nonlocality, in the course of which we will introduce the Bell inequalities – inequalities that hold for all states admitting an LHV model. These inequalities, when interpreted geometrically, define a convex polytope, which will be constructed in Chapter 4. In Chapter 5 we will show how to use symmetry transformations to group the inequalities into equivalence classes while in Chapter 6 we will introduce the new method announced above. Finally, we will apply the results from the preceding Chapters to a particular set of inequalities in Chapter 7 and conclude the thesis in Chapter 8.

¹See Section 3.2.1 for some references.

²See Section 3.2 for a detailed characterisation of LHV models.

2. Quantum Mechanical Formalism

The quantum mechanical formalism can be summarised in four postulates. In this chapter we first motivate these postulates for systems whose state is known completely in Section 2.1 and then extend it to systems whose state is known only within some level of uncertainty in Section 2.2, to allow for a more refined description.

2.1. Postulates of Quantum Mechanics

2.1.1. State Space

Quantum mechanics is written in the language of linear algebra, the field of vector spaces and linear transformations. The state of any quantum mechanical system is represented by a vector in a Hilbert space \mathcal{H} of possibly infinite dimension. The restriction to Hilbert spaces ensures that any Cauchy sequence of vectors converges and provides us with an inner product, denoted $\langle \cdot | \cdot \rangle$, to compute the lengths of the vectors. All vectors $|\psi\rangle$ representing a quantum mechanical system are normalised to unit length: $\langle \psi | \psi \rangle = |\psi|^2 = 1$. Together, these requirements constitute the first postulate of quantum mechanics:

Postulate 1. *Each quantum mechanical system is described by a unit vector $|\psi\rangle$ in a Hilbert space \mathcal{H} . This vector is called the wavefunction of the system. [NC00, p.80]*

2.1.2. Evolution

Given the state of the system, one would also like to describe its dynamics. The evolution equation for a closed quantum system was discovered by Erwin Schrödinger in 1926 and has been verified by a great number of experiments. Yet it cannot be derived rigorously from first principles. Therefore we have to add a second postulate that determines the time evolution of the wavefunction.

Postulate 2. *The time evolution of the wavefunction is given by Schrödinger's equation:*

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle \quad (2.1)$$

where \hat{H} is a hermitian operator ($\hat{H} = \hat{H}^\dagger$) known as the Hamiltonian of the system and $\hbar = \frac{h}{2\pi} = 1.054... \text{ Js}$ is the experimentally determined reduced Planck constant. [NC00, p.82]

As Schrödinger's equation is a linear ordinary differential equation of first order, its solution is given by the exponential:

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$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} |\psi(t_0)\rangle \quad (2.2)$$

The linearity of Schrödinger's equation also implies that any linear combination $\sum_i |\psi\rangle^{(i)}$ of solutions $|\psi\rangle^{(i)}$ solves the equation as well. This linear combination is usually called a *superposition of wavefunctions* and the fact that each superposition is a solution itself is known as the *superposition principle*.

The form 2.2 of the general solutions to Schrödinger's equation also allows us to express the time evolution of any system in a different way. By defining the unitary operator

$$U(t, t_0) \equiv e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}(t-t_0) \right)^n \frac{\hat{H}^n}{n!} \quad (2.3)$$

the time evolution can be described with

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle. \quad (2.4)$$

No matter which expression one uses, finding the actual Hamiltonian or unitary operator for a given system plus solving the corresponding differential equation is quite a complex problem. However, the exact form of \hat{H} will be of no concern to us in the following discussion.

2.1.3. Measurements

We also want to describe measurements on a given system.¹ The behaviour of the wavefunction during a measurement is described by

Postulate 3. *Measurements on a quantum system are described by a set of operators $\{M_m\}$ acting on the system's wavefunction, with the index m indicating the possible outcomes of the measurement. These measurement operators satisfy $\sum_m M_m^\dagger M_m = \mathbb{1}$. The probability that upon measuring a given wavefunction $|\psi\rangle$ the outcome is m is*

$$p(m) = \langle \psi | M_m^\dagger M_m | \psi \rangle \quad (2.5)$$

and the state after the measurement is

$$|\psi'\rangle = \frac{M_m |\psi\rangle}{\sqrt{p(m)}}. \quad (2.6)$$

[NC00, p.84-85]

¹It is a strange feature of quantum mechanics that one has to make an additional postulate about measurements. The measurement apparatuses are, after all, quantum systems themselves, so one should be able to describe them in the same way as the system being measured. Yet experiments such as the Stern-Gerlach-experiment suggest that there is something fundamentally different about the measurement process. Lots of discussion has been devoted to this *measurement problem* and still no consensus has been found.

2. Quantum Mechanical Formalism

If one defines $E_m \equiv M_m^\dagger M_m$, one obtains a *positive-operator valued measure (POVM)* - a set of hermitian, positive-semidefinite² operators $\{E_m\}$ satisfying $\sum_m E_m = \mathbb{1}$. A special class of POVMs are projective measurements.

Projective measurement. *A projective measurement is described by a hermitian operator $M = M^\dagger$, called an observable, which can be written as*

$$M = \sum_m \lambda_m |m\rangle\langle m| \quad (2.7)$$

where $\{|m\rangle\}$ is an orthonormal basis of eigenvectors of M satisfying $\langle m|m'\rangle = \delta_{mm'}$ and λ_m are the corresponding eigenvalues. The probability of obtaining the outcome λ_m is

$$p(m) = \langle \psi|m\rangle \langle m|\psi\rangle = |\langle m|\psi\rangle|^2 \quad (2.8)$$

and the state after the measurement is

$$|\psi'\rangle = \frac{|m\rangle\langle m|\psi\rangle}{\sqrt{|\langle m|\psi\rangle|^2}} = |m\rangle. \quad (2.9)$$

This is actually quite intuitive - after measuring the outcome λ_m we can be sure that the system is in the corresponding state $|m\rangle$. Let's look at an example to illustrate this.

We want to measure the spin of an electron in a given direction. There are two orthonormal spin-states: $|\uparrow\rangle$ and $|\downarrow\rangle$ satisfying $\langle \uparrow|\uparrow\rangle = \langle \downarrow|\downarrow\rangle = 1$ and $\langle \uparrow|\downarrow\rangle = 0$. The measurement apparatus gives out $+1$ if the electron has spin up and -1 if the electron has spin down. The corresponding measurement operator is

$$M = +1 \cdot |\uparrow\rangle\langle \uparrow| - 1 \cdot |\downarrow\rangle\langle \downarrow| \quad (2.10)$$

Let's say the electron is in the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Then the probability for each of the two outcomes is

$$p(\uparrow) = |\langle \uparrow|\psi\rangle|^2 = \frac{1}{2} \quad p(\downarrow) = |\langle \downarrow|\psi\rangle|^2 = \frac{1}{2} \quad (2.11)$$

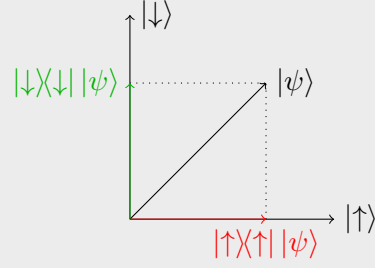
Now let's assume that the measurement apparatus showed the result $+1$. Intuitively we would conclude that the system is in the spin-up-state $|\uparrow\rangle$. This intuition is met by postulate 3: the post-measurement state is

$$|\psi'\rangle = \frac{|\uparrow\rangle\langle \uparrow|\psi\rangle}{\sqrt{p(\uparrow)}} = |\uparrow\rangle \quad (2.12)$$

²A hermitian operator A acting on \mathcal{H} is positive-semidefinite, denoted $A \succeq 0$, if and only if $\forall |\phi\rangle \in \mathcal{H} : \langle \phi|A|\phi\rangle \geq 0$.

2. Quantum Mechanical Formalism

One can also say that after the measurement the wavefunction is *projected* onto the measured state. This is illustrated by the figure on the right.



2.1.4. Composite Systems

Finally, we ask for a way to describe the composition of two or more quantum mechanical systems. As the systems are described by wavefunctions in a Hilbert space, we need a way to join Hilbert spaces and their inhabitants:

$$\mathcal{H}_{AB} = \mathcal{H}_A \circ \mathcal{H}_B \quad |\psi_{AB}\rangle = |\psi_A\rangle \circ |\psi_B\rangle \in \mathcal{H}_{AB} \quad (2.13)$$

Ideally, not only the joint wavefunctions but also any superposition $\sum_i \alpha_i |\psi_{AB}\rangle^{(i)}$ of joint wavefunctions would be part of the joint Hilbert space - after all, this is the case for the wavefunctions of single systems. These requests are met by the *tensor product* [TiB16].

Definition 1. Let \mathcal{H}_A and \mathcal{H}_B be two Hilbert spaces. Then the algebraic tensor product consists of the formal finite sums

$$\sum_{i,j} a_i \otimes b_j \text{ where } a_i \in \mathcal{H}_A, b_j \in \mathcal{H}_B. \quad (2.14)$$

If \mathcal{H}_A and \mathcal{H}_B are finite-dimensional spaces, the above construction defines the tensor product Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. Otherwise the algebraic tensor product has to be completed in order to obtain a Hilbert space.

The computation rules for $a, a_i \in \mathcal{H}_A$, $b, b_i \in \mathcal{H}_B$ and $\lambda \in \mathbb{C}$ are as follows:

$$(a_1 + a_2) \otimes b = a_1 \otimes b + a_2 \otimes b$$

$$a \otimes (b_1 + b_2) = a \otimes b_1 + a \otimes b_2$$

$$(\lambda a) \otimes b = \lambda(a \otimes b)$$

$$a \otimes (\lambda b) = \lambda(a \otimes b)$$

and the inner product is

$$\left\langle \sum_{i,j} a_i \otimes b_j \left| \sum_{k,l} c_k \otimes d_l \right. \right\rangle_{\mathcal{H}_A \otimes \mathcal{H}_B} = \sum_{i,j,k,l} \langle a_i | c_k \rangle_{\mathcal{H}_A} \langle b_j | d_l \rangle_{\mathcal{H}_B} \quad (2.15)$$

with $c_k \in \mathcal{H}_A$ and $d_l \in \mathcal{H}_B$.

2. Quantum Mechanical Formalism

Equipped with a way to join Hilbert spaces, we can make the following postulate:

Postulate 4. *Let A and B be two physical systems with corresponding wavefunctions $|\psi_A\rangle \in \mathcal{H}_A$ and $|\psi_B\rangle \in \mathcal{H}_B$. Then the composite system of A and B is described by the wavefunction $|\psi_A\rangle \otimes |\psi_B\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$.*

If one has two operators \hat{A} and \hat{B} acting on \mathcal{H}_A and \mathcal{H}_B respectively, the action of the joint operator $\hat{A} \otimes \hat{B}$ acting on $\mathcal{H}_A \otimes \mathcal{H}_B$ is defined by

$$(\hat{A} \otimes \hat{B})(|\psi_A\rangle \otimes |\psi_B\rangle) = \hat{A}|\psi_A\rangle \otimes \hat{B}|\psi_B\rangle. \quad (2.16)$$

[NC00, p.94]

For example, let the wavefunctions of the component-systems be $|\psi_A\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and $|\psi_B\rangle = |\uparrow\rangle$. Then the composite system can be described by the wavefunction

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\uparrow\rangle + |\downarrow\rangle \otimes |\uparrow\rangle) = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle) \quad (2.17)$$

with the short-hand notation $|a\rangle \otimes |b\rangle = |ab\rangle$.

If one conducts a measurement M_A on system A while leaving system B invariant, the corresponding measurement operator is $M = M_A \otimes \mathbb{1}$ and its action upon the wavefunction of the composite system is

$$M|\psi_{AB}\rangle = M_A \left[\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \right] \otimes |\uparrow\rangle. \quad (2.18)$$

2.2. Ensembles of States

The aforementioned postulates of quantum mechanics allow us to fully describe a given system or composition of systems with a single wavefunction. In experiments, however, this wavefunction is often known only within a level of uncertainty.

For example, an experimenter might try to prepare 100 photons in the polarisation state $|\psi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Unfortunately the apparatus he uses to prepare the particles is not very exact and prepares 25 of the photons in a different state, $|\psi_2\rangle = |\uparrow\rangle$. In this case the experimenter only knows the possible states $|\psi_1\rangle$ and $|\psi_2\rangle$ and their respective probabilities $p_1 = \frac{3}{4}$ and $p_2 = \frac{1}{4}$.

If there is no way to avoid these uncertainties, we need a new formalism that describes not only wavefunctions and their behaviour, but also the probabilities associated with them - a so-called *ensemble of states* $\{|\psi_i\rangle, p_i\}$. This formalism should reproduce the results we obtained so far for *pure states*, i.e. ensembles where the state of the system is

2. Quantum Mechanical Formalism

known with certainty, yet allow us to include the uncertainties for any other state. We will see, that the *density operator* meets these requirements in quite an intuitive way.³

2.2.1. Density operators

Definition 2. *The density operator $\hat{\rho}$ describing the ensemble $\{|\psi_i\rangle, p_i\}$ is given by*

$$\hat{\rho} \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad (2.19)$$

Given an arbitrary orthonormal basis $\{|i\rangle\}_{i=1,\dots,n}$ one can represent $\hat{\rho}$ with a matrix, the so-called density matrix ρ , with entries

$$\rho_{ij} = \langle i|\hat{\rho}|j\rangle \quad (2.20)$$

Property 1. *$\hat{\rho}$ is hermitian.*

$$\hat{\rho}^\dagger = \sum_i p_i (|\psi_i\rangle\langle\psi_i|)^\dagger = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \hat{\rho} \quad (2.21)$$

Property 2. *$\hat{\rho}$ is a positive-semidefinite operator, i.e. $\forall\phi \in \mathcal{H} : \langle\phi|\hat{\rho}|\phi\rangle \geq 0$.*

$$\langle\phi|\hat{\rho}|\phi\rangle = \sum_i p_i \langle\phi|\psi_i\rangle \langle\psi_i|\phi\rangle = \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0 \quad (2.22)$$

Property 3. *$\hat{\rho}$ has unit trace.*

$$\text{Tr}(\hat{\rho}) = \sum_i p_i \text{Tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i p_i \text{Tr}(\langle\psi_i|\psi_i\rangle) = \sum_i p_i = 1 \quad (2.23)$$

So in the example above, the ensemble is given by

$$\{|\psi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle), p_1 = \frac{3}{4}, |\psi_2\rangle = |\uparrow\rangle, p_2 = \frac{1}{4}\} \quad (2.24)$$

and therefore the density operator is

$$\hat{\rho} = \frac{3}{4} |\psi_1\rangle\langle\psi_1| + \frac{1}{4} |\psi_2\rangle\langle\psi_2| = \frac{5}{8} |\uparrow\rangle\langle\uparrow| + \frac{3}{8} (|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) \quad (2.25)$$

If we choose $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ as a basis, the corresponding density matrix is

$$\rho = \frac{5}{8} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{3}{8} \left[\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right] = \frac{1}{8} \begin{pmatrix} 5 & 3 \\ 3 & 3 \end{pmatrix} \quad (2.26)$$

³The presentation in the next section is based on [NC00, p.98-102].

2. Quantum Mechanical Formalism

The density operator allows us to reformulate the postulates of quantum mechanics for ensembles of states. The first postulate becomes

Postulate 1'. *Each quantum mechanical ensemble is described by a density operator $\hat{\rho} \in \mathcal{B}(\mathcal{H})$ where $\mathcal{B}(\mathcal{H})$ describes the space of bounded linear operators acting on \mathcal{H} .*

For describing the time evolution of the system, it makes sense to assume that the probabilities associated with each state do not change over time. Additionally, if we want to reproduce the results from Section 2.1, all state vectors have to evolve according to equation 2.3. Inserting this into the definition for density operators and using the short-hand notation $U(t, t_0) \equiv U$ we obtain

$$\begin{aligned} \hat{\rho}(t) &= \sum_i p_i |\psi_i(t)\rangle\langle\psi_i(t)| = \sum_i p_i U |\psi_i(t_0)\rangle\langle\psi_i(t_0)| U^\dagger \\ &= U \left[\sum_i p_i |\psi_i(t_0)\rangle\langle\psi_i(t_0)| \right] U^\dagger = U \hat{\rho}(t_0) U^\dagger, \end{aligned} \tag{2.27}$$

so the second postulate becomes

Postulate 2'. *The time evolution of the density operator is given by*

$$\hat{\rho}(t) = U(t, t_0) \hat{\rho}(t_0) U(t, t_0)^\dagger \tag{2.28}$$

where $U(t, t_0)$ is a unitary operator.

To find a description for measurements on density operators, we make use of our intuition about probabilities. If we know the conditional probability $p(m|i)$ of obtaining a result m , given the state $|\psi_i\rangle$, then the probability of obtaining this result in an ensemble of states $\{|\psi_i\rangle, p_i\}$ must be the sum of the conditional probabilities $p(m|i)$ weighed with the probability that the system actually is in the state $|\psi_i\rangle$.⁴ More formally:

$$\begin{aligned} p(m) &= \sum_i p_i p(m|i) \stackrel{2.5}{=} \sum_i p_i \text{Tr}(\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle) \\ &= \sum_i p_i \text{Tr}(\underbrace{M_m^\dagger M_m}_{\equiv \hat{M}_m} |\psi_i\rangle\langle\psi_i|) = \text{Tr}(\hat{M}_m \hat{\rho}) \end{aligned} \tag{2.29}$$

where in the first line we used that the trace of a number is just the number itself. This way the third postulate turns into

Postulate 3'. *Measurements on an ensemble of states are described by a set of positive-semidefinite measurement operators $\{\hat{M}_m\}$ acting on the system's density operator. These measurement operators satisfy $\sum_m \hat{M}_m = \mathbf{1}$. The probability that upon measuring a given system with density operator $\hat{\rho}$ the outcome is m is*

$$p(m) = \text{Tr}(\hat{M}_m \hat{\rho}). \tag{2.30}$$

⁴This is also known as the “law of total probability”.

2. Quantum Mechanical Formalism

Finally, to combine ensembles of states, we simply use the tensor product as well.

Postulate 4'. *Let A and B be two physical systems with corresponding density operators $\hat{\rho}_A \in \mathcal{B}(\mathcal{H}_A)$ and $\hat{\rho}_B \in \mathcal{B}(\mathcal{H}_B)$. Then the composite system of A and B is described by the density operator $\hat{\rho}_A \otimes \hat{\rho}_B \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$.*

The action of a joint operator continues to be defined by equation 2.16.

2.2.2. Partial Trace

Given the density operator for a composite system, we can use the partial trace to find descriptions for its subsystems.

Definition 3. *The partial trace is a linear map defined by*

$$\text{Tr}_A : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_B) \qquad \text{Tr}_B : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_A) \qquad (2.31)$$

$$A \otimes B \mapsto \text{Tr}(A) \cdot B \qquad A \otimes B \mapsto A \cdot \text{Tr}(B) \qquad (2.32)$$

and extended by linearity to any operator $\hat{\rho} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$.

The partial trace of a density operator shows an interesting feature when it comes to measurements. If one performs a measurement $M = \mathbb{1} \otimes M_B$ on a composite system described by $\hat{\rho}_{AB}$ then this gives the same statistics as performing the measurement M_B on the partial trace $\text{Tr}_A(\hat{\rho}_{AB})$. This can easily be seen for product states $\hat{\rho}_{AB} = \hat{\rho}_A \otimes \hat{\rho}_B$:

$$p(m) = \text{Tr}(M\hat{\rho}_{AB}) = \text{Tr}(\mathbb{1}\hat{\rho}_A \otimes M_B\hat{\rho}_B) = \underbrace{\text{Tr}(\hat{\rho}_A)}_{=1} \text{Tr}(M_B\hat{\rho}_B) = \text{Tr}(M_B\hat{\rho}_B) \qquad (2.33)$$

and generalises to arbitrary states $\hat{\rho}_{AB} = \sum_i p_{ij}^{kl} |a_i\rangle\langle a_j| \otimes |b_k\rangle\langle b_l|$.⁵

So via applying the partial trace on A , we obtain a density operator that describes correctly how subsystem B behaves under measurement. This density operator is called the *reduced density operator*

$$\hat{\rho}_B \equiv \text{Tr}_A(\hat{\rho}_{AB}) \qquad (2.34)$$

and the process of applying the partial trace on A is often referred to as *tracing out system A* . The same argument can be repeated for the reduced density operator for system A with

$$\hat{\rho}_A \equiv \text{Tr}_B(\hat{\rho}_{AB}). \qquad (2.35)$$

⁵See appendix A for the full proof.

2. Quantum Mechanical Formalism

As an example, let's look at the density operator corresponding to a perfect mixture ($p_1 = p_2 = \frac{1}{2}$) of $|\psi_1\rangle = |\uparrow\rangle \otimes |\uparrow\rangle$ and $|\psi_2\rangle = |\downarrow\rangle \otimes |\uparrow\rangle$:

$$\hat{\rho}_{AB} = \frac{1}{2} |\uparrow\rangle\langle\uparrow| \otimes |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow| \otimes |\uparrow\rangle\langle\uparrow| \quad (2.36)$$

Tracing out system A gives

$$\hat{\rho}_B = \frac{1}{2} \underbrace{\text{Tr}(|\uparrow\rangle\langle\uparrow|)}_{=1} \otimes |\uparrow\rangle\langle\uparrow| + \frac{1}{2} \underbrace{\text{Tr}(|\downarrow\rangle\langle\downarrow|)}_{=1} \otimes |\uparrow\rangle\langle\uparrow| = |\uparrow\rangle\langle\uparrow| \quad (2.37)$$

This is what we would have expected - after all, system B is always in the up-state. Tracing out system B , on the other hand, gives

$$\hat{\rho}_A = \frac{1}{2} |\uparrow\rangle\langle\uparrow| \otimes \underbrace{\text{Tr}(|\uparrow\rangle\langle\uparrow|)}_{=1} + \frac{1}{2} |\downarrow\rangle\langle\downarrow| \otimes \underbrace{\text{Tr}(|\uparrow\rangle\langle\uparrow|)}_{=1} = \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow|, \quad (2.38)$$

which corresponds to a perfect mixture of up- and down-states.

The concept of reduced density matrices will be particularly useful when it comes to characterising entanglement.

3. Entanglement & Nonlocality

In this chapter we will discuss the relation between two central concepts in quantum mechanics: entanglement and nonlocality. We will see that some entangled states do not admit a local hidden variable model - a fact that has puzzled many great minds since the early days of quantum mechanics - and investigate the properties of these states.

3.1. Entanglement

Entanglement is defined via separability: A state is entangled if and only if it is not separable. Separability, in turn, is defined as follows:

Definition 4. A state $\hat{\rho} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is called separable if there exist density operators $\hat{\rho}_A^{(i)} \in \mathcal{B}(\mathcal{H}_A)$, $\hat{\rho}_B^{(i)} \in \mathcal{B}(\mathcal{H}_B)$ and probabilities p_i such that

$$\hat{\rho} = \sum_i p_i \hat{\rho}_A^{(i)} \otimes \hat{\rho}_B^{(i)}. \quad (3.1)$$

Entangled subsystems cannot be described individually - one always has to consider the entire system $\hat{\rho}$. This is illustrated in the following example.

Let's assume that a system is in the pure entangled state $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$.¹The corresponding density matrix is

$$\hat{\rho}_{AB} = |\phi^+\rangle\langle\phi^+| = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 11|) \quad (3.2)$$

Now we want to know the state of the subsystem A, so we trace out system B and obtain

$$\hat{\rho}_A = \text{Tr}_B(\hat{\rho}_{AB}) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \quad (3.3)$$

The reduced density operator tells us that system A is in a perfect mixture of the states $|0\rangle$ and $|1\rangle$ - despite the fact that the composite system was in a pure state! Even though the state of the composite system was fully known, we cannot say, whether system A is in state $|0\rangle$ or $|1\rangle$.

One can easily see that results of this kind can exclusively be obtained with entangled states. If a pure state is separable, it can be written as $|\psi\rangle = |\psi_A\rangle|\psi_B\rangle$ and the reduced density matrices are $\hat{\rho}_A = |\psi_A\rangle\langle\psi_A|$ resp. $\hat{\rho}_B = |\psi_B\rangle\langle\psi_B|$, both of which correspond to pure states.

¹We will later see a proof that this state actually *is* entangled.

3.1.1. The Separability Problem

It is not always easy to figure out if a given state is separable. In fact, it has been shown that detecting separability is in general NP-hard [Gur03]. We can, however, find criteria for separability. In this thesis we will focus on one particular criterion, which was first discovered by Horodecki and Peres [HHH96, Per96]. It relies on two concepts: positive, but not completely positive maps [TiB16] and the partial transposition.

Definition 5. A map $\Lambda: \mathcal{B}(\mathcal{H}_1) \rightarrow \mathcal{B}(\mathcal{H}_2)$ is positive if for all $\rho \in \mathcal{B}(\mathcal{H}_1)$ ²

$$\rho \succeq 0 \Rightarrow \Lambda[\rho] \succeq 0. \quad (3.4)$$

Definition 6. A map $\Lambda: \mathcal{B}(\mathcal{H}_1) \rightarrow \mathcal{B}(\mathcal{H}_2)$ is completely positive if for all $n \in \mathbb{N}$ and all $\rho \in \mathbb{C}^n \otimes \mathcal{B}(\mathcal{H}_1)$

$$\rho \succeq 0 \Rightarrow (\mathbb{1}_n \otimes \Lambda)[\rho] \succeq 0. \quad (3.5)$$

Note that to describe a physical system, ρ has to be positive semi-definite. While a positive map preserves this property when applied to the whole system, it does not necessarily preserve it when applied to one of the subsystems only. Therefore the application of a positive map is not always a physical operation. A completely positive map, on the other hand, preserves positive semi-definiteness, no matter which subsystem it is applied to. To ensure that all of the requirements for density operators in Definition 2 are met, a physical operation has to correspond to a completely positive map Λ that does not change the trace or hermiticity of the state it acts on.

Equipped with the definitions above, we can show an interesting relation between separable states and the action of positive maps. Let Λ be a positive but not necessarily completely positive map on $\mathcal{B}(\mathcal{H}_A)$ and $\mathcal{B}(\mathcal{H}_B)$. Furthermore, consider a separable state $\rho_{AB} = \sum_i p_i \rho_A^{(i)} \otimes \rho_B^{(i)}$ where $\rho_A^{(i)} \in \mathcal{B}(\mathcal{H}_A)$ and $\rho_B^{(i)} \in \mathcal{B}(\mathcal{H}_B)$ for all i . Because Λ is a positive map, it preserves the positive semi-definiteness of every $\rho_A^{(i)}$ and $\rho_B^{(i)}$. If we now apply $(\mathbb{1}_n \otimes \Lambda)$ to ρ_{AB} , we obtain

$$\begin{aligned} (\mathbb{1}_n \otimes \Lambda)[\rho_{AB}] &= (\mathbb{1}_n \otimes \Lambda) \left[\sum_i p_i \rho_A^{(i)} \otimes \rho_B^{(i)} \right] \\ &= \sum_i p_i \rho_A^{(i)} \otimes \Lambda[\rho_B^{(i)}] \succeq 0 \end{aligned} \quad (3.6)$$

where the last inequality follows from the fact that $\Lambda[\rho_B^{(i)}] \succeq 0$ for all i . So a necessary criterion for separability is that any positive map on ρ is also completely positive. To obtain the Peres-Horodecki criterion, we have to identify Λ with the transposition with respect to the computational basis. Then the action on one of the subsystems, $(\mathbb{1}_n \otimes \Lambda)$, corresponds to the partial transpose.

²From now on we will consider only the matrix representation of density operators.

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Definition 7. The partial transpose T_A resp. T_B is a linear map defined by

$$T_A : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \quad T_B : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \quad (3.7)$$

$$A \otimes B \mapsto A^T \otimes B \quad A \otimes B \mapsto A \otimes B^T \quad (3.8)$$

and extended by linearity to any operator $\hat{\rho} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$. The transposition of a matrix

$$A = (a_{ij})_{ij} = \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{m1} & \dots & a_{mn} \end{pmatrix} \in \mathbb{C}^{m \times n}$$

is defined by

$$A^T = (a_{ij})_{ji} = \begin{pmatrix} a_{11} & \dots & a_{m1} \\ \vdots & & \vdots \\ a_{1n} & \dots & a_{mn} \end{pmatrix} \in \mathbb{C}^{n \times m}. \quad (3.9)$$

The resulting criterion is often also called *PPT-criterion*, where PPT stands for “positive partial transpose”, and can be summarised as follows.

PPT-Criterion. If a state is separable, then its partially transposed density matrix is positive-semidefinite, i.e. $\rho_{AB}^{T_B} \succeq 0$.

It has been shown that for systems with dimension 2×2 and 2×3 this criterion is also sufficient. In general, however, this is not the case [HHH96].

We can now show, that the state $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ from our previous example is indeed entangled. The matrix representations of ρ_{AB} and its partial transpose on B are:

$$\rho_{AB} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \quad \rho_{AB}^{T_B} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (3.10)$$

To check if $\rho_{AB}^{T_B}$ is positive-semidefinite we calculate its eigenvalues and obtain

$$\lambda_1 = -1, \quad \lambda_2 = \lambda_3 = \lambda_4 = 1 \quad (3.11)$$

This means that $\langle v_1 | \rho_{AB}^{T_B} | v_1 \rangle = \lambda_1 < 0$, where $|v_1\rangle$ is the eigenvector corresponding to λ_1 . Therefore $\rho_{AB}^{T_B}$ is not positive-semidefinite and the state must be entangled.

3.2. Nonlocality

The second concept we want to discuss in this section is nonlocality. Nonlocality arises when two distant events influence each other within a very short amount of time. More precisely, in a local theory spacelike-separated events cannot influence each other. Two points in spacetime, (ct_1, \mathbf{x}_1) and (ct_2, \mathbf{x}_2) , are spacelike-separated if the spatial distance $\Delta x \equiv \|\mathbf{x}_2 - \mathbf{x}_1\|$ is greater than the distance light travels within the time interval $\Delta t \equiv t_2 - t_1$ (see Figure 3.1). For example, an event on Mars at 12:00 am cannot locally influence an event on earth at 12:01 am because it takes light at least three minutes to travel from one planet to the other.

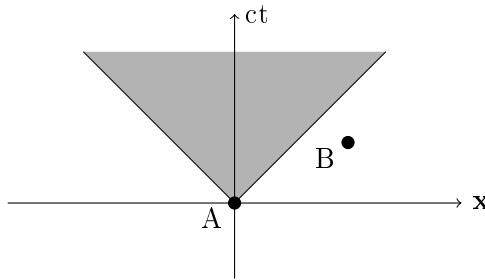


Figure 3.1.: Two spacelike-separated events A and B. The diagonal lines represent the path of light in spacetime, so event A can only locally influence events within the shaded area, the so-called *light cone*. Any events outside its light cone are spacelike-separated from A.

For a long time locality was assumed to be a fundamental property of nature. In 1964, however, John Bell showed that quantum mechanics violates this property and proposed an experiment to test if these quantum mechanical predictions are true [Bel64]. And indeed, when Aspect conducted the first *Bell experiment* in 1982, the experimental results agreed perfectly with the theoretical predictions [AGR81]. Since then many more experiments have been conducted, closing several loopholes and confirming Aspect's results.³

3.2.1. The CHSH inequality

Instead of following Bell's original proof, we will look at a more instructive generalisation first presented by Clauser, Horne, Shimony and Holt in 1969 [CHSH69]. Their argument is based on the setting illustrated in figure 3.2. A pair of entangled photons in the state

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad (3.12)$$

³See, for example, the three Bell tests conducted independently in 2015 by Hensen [HBD⁺15], Giustina [GVW⁺15] and Shalm [SMSC⁺15] and the work of the group around Harald Weinfurter at LMU [PBD⁺00].

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is generated in the grey box and sent to two distant observers, Alice and Bob. Both of them can choose between two different measurements, A_0, A_1 and B_0, B_1 respectively.

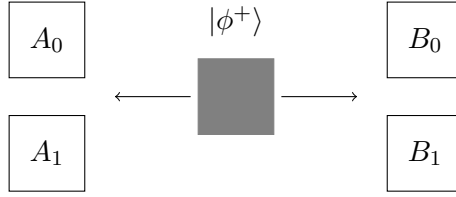


Figure 3.2.: Setting for the CHSH-scenario.

For example, A_0 and B_0 could correspond to measurements of the polarisation in x-direction while A_1 and B_1 correspond to the same measurements in z-direction. In general, however, this argument is independent of the explicit form of the measurement operators. In the CHSH-setting each of the measurements has two outcomes, $+1$ and -1 , which will be denoted by $a, b \in \{+1, -1\}$. The choice of measurement will be represented by $x \in \{0, 1\}$ for Alice and $y \in \{0, 1\}$ for Bob. Now Alice and Bob run the experiment many times with random measurement settings, each time obtaining a pair of outcomes a and b .

a_0	a_1	b_0	b_1
+1		-1	
-1			-1
	+1	-1	
-1			-1
	+1		+1
⋮	⋮	⋮	⋮

Figure 3.3.: A typical protocol of the Bell experiment.

The outcomes are governed by a probability distribution $p(ab|xy)$ depending on the choice of measurements xy . In the following argument we will invoke the locality principle to further specify this probability distribution. This way we can derive a simple inequality that has to hold for any state describable with a local hidden variable model, yet can be violated by nonlocal states. We then show that for the particular quantum state $|\phi^+\rangle$ this inequality is violated and conclude that quantum mechanics is nonlocal.

As mentioned before, locality implies that two distant events cannot influence each other instantaneously. So, let's assume that Alice and Bob are arbitrarily far apart and perform their measurements within a very short time frame - so short that no signal can be transmitted locally between the two measurements. They also do not decide, which measurement they are going to perform, until *very* shortly before the actual measurement. So, if they are far enough apart, Alice's choice of measurement cannot locally influence

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Bob's result and vice versa. More formally, the probabilities for a and b have to be independent of the distant measurement: $p(ab|xy) = p(a|x)p(b|y)$. However, one has to take into account that there might be some other factors, the so-called *hidden variables* λ , that influence both Alice's and Bob's result. The possible values of the hidden variables are governed by a normalised probability distribution $q(\lambda)$, which will not be specified further to keep the results as general as possible. Considering these hidden variables the probability distribution takes the form

$$p(ab|xy) = \int_{\Lambda} d\lambda q(\lambda) p(a|x, \lambda) p(b|y, \lambda). \quad (3.13)$$

Models that can be described with this kind of probability distributions are called *local-hidden-variable (LHV) models*.

Let's now consider the following quantity:

$$\langle B \rangle = \langle A_0 B_0 \rangle + \langle A_0 B_1 \rangle + \langle A_1 B_0 \rangle - \langle A_1 B_1 \rangle \quad (3.14)$$

where the expectation value $\langle \cdot \rangle$ is defined as $\langle A \rangle \equiv \sum_{i=1}^n p(a_i, \lambda) a_i$ with a_i being the possible outcomes of A and $p(a_i, \lambda)$ the respective normalised probabilities. Therefore

$$\begin{aligned} \langle B \rangle &= \int_{\Lambda} d\lambda q(\lambda) (\langle A_0 \rangle \langle B_0 \rangle + \langle A_0 \rangle \langle B_1 \rangle + \langle A_1 \rangle \langle B_0 \rangle - \langle A_1 \rangle \langle B_1 \rangle)_{\lambda} \\ &\leq \int_{\Lambda} d\lambda q(\lambda) (|\langle A_0 \rangle| |\langle B_0 \rangle + \langle B_1 \rangle| + |\langle A_1 \rangle| |\langle B_0 \rangle - \langle B_1 \rangle|)_{\lambda} \end{aligned} \quad (3.15)$$

where the second line follows from the triangle inequality. Because of $a_i \in \{-1, +1\}$ $|\langle A_0 \rangle|, |\langle A_1 \rangle| \leq 1$ holds and the inequality simplifies to

$$S \leq \int_{\Lambda} d\lambda q(\lambda) (|\langle B_0 \rangle + \langle B_1 \rangle| + |\langle B_0 \rangle - \langle B_1 \rangle|)_{\lambda} \quad (3.16)$$

It can be seen by case differentiation with respect to the extremal values $+1$ and -1 of $\langle B_0 \rangle$ and $\langle B_1 \rangle$ that no matter which value one chooses for the expectation values the expression $|\langle B_0 \rangle + \langle B_1 \rangle| + |\langle B_0 \rangle - \langle B_1 \rangle|$ is always less than or equal to two. Therefore

$$\langle B \rangle \leq 2 \int_{\lambda} d\lambda q(\lambda) = 2. \quad (3.17)$$

This is the so-called *CHSH-inequality*:

$$\boxed{\langle A_0 B_0 \rangle + \langle A_0 B_1 \rangle + \langle A_1 B_0 \rangle - \langle A_1 B_1 \rangle \leq 2} \quad (3.18)$$

Any probability distribution that can be described by a local hidden variable model must satisfy this inequality.

Finally, we take a look at a particular set-up [KS11]. Alice and Bob both want to measure the polarisation of their photon in two directions. A polarisation measurement

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in an arbitrary direction $\mathbf{r} = (\sin(\alpha), \cos(\alpha))^T$ in the x-z-plane can be represented by the operator

$$\hat{O} = \sin(\alpha)\sigma_x + \cos(\alpha)\sigma_z = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ \sin(\alpha) & -\cos(\alpha) \end{pmatrix} \quad (3.19)$$

where σ_x and σ_z are Pauli matrices. While Alice measures the polarisation of her photon in x- and z-direction, Bob's polarisation filters are shifted by 45° (see figure 3.4).

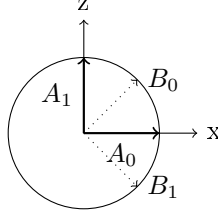


Figure 3.4.: Directions of Alice's and Bob's measurements.

So Alice's and Bob's measurements are

$$A_0 = \hat{O}(0) \quad B_0 = \hat{O}(\pi/4) \quad (3.20)$$

$$A_1 = \hat{O}(\pi/2) \quad B_1 = \hat{O}(-\pi/4) \quad (3.21)$$

As mentioned in the beginning of this section, the photons are in the state $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, so the quantum mechanical expectation value can be computed via

$$\langle A_i B_j \rangle = \langle \phi^+ | A_i \otimes B_j | \phi^+ \rangle. \quad (3.22)$$

The results are: $\langle A_0 B_0 \rangle = \langle A_0 B_1 \rangle = \langle A_1 B_0 \rangle = \frac{1}{\sqrt{2}}$ and $\langle A_1 B_1 \rangle = -\frac{1}{\sqrt{2}}$ and therefore

$$\langle B \rangle = \langle A_0 B_0 \rangle + \langle A_0 B_1 \rangle + \langle A_1 B_0 \rangle - \langle A_1 B_1 \rangle = 2\sqrt{2} > 2 \quad (3.23)$$

This is clearly a violation of the CHSH-inequality from which we conclude that quantum mechanics is indeed nonlocal.

Bell Inequalities in General

The CHSH inequality is just one of many *Bell Inequalities* indicating nonlocality in quantum mechanics. One can generalise the simple scenario of two parties (Alice and Bob) and two measurement apparatuses (spin in x- and y-direction) with two possible outcomes (+1, -1) to settings of n parties and m measurement apparatuses with d possible outcomes. Such a setting will be described by the triplet of numbers (n, m, d) in this thesis. In Chapter 4 we will discuss a way to generate the Bell inequalities for a given scenario. For now it is enough to bear in mind that the CHSH-inequality is just one specimen in a whole zoo of Bell inequalities.

3.3. The Peres Conjecture

In our discussion so far we may have used entanglement to show that quantum mechanics is nonlocal but we have yet to show that entanglement is actually the decisive factor when it comes to nonlocality. In Section 3.2.1 we already argued that the locality condition manifests itself in the following equation:

$$p(ab|xy) = \int_{\Lambda} d\lambda q(\lambda) p(a|x, \lambda) p(b|y, \lambda) \quad (3.24)$$

It can be seen quite easily that any separable state satisfies this condition: Suppose we perform a measurement $M = M_{A|x} \otimes M_{B|y}$ on a composite system in a separable state $\hat{\rho}_{AB}$ where x and y indicate the choice of the measurement apparatus on each site. Due to the third postulate, the probabilities of the possible outcomes are given by

$$\begin{aligned} p(ab|xy) &= \text{Tr}(M \hat{\rho}_{AB}) = \text{Tr}\left[(M_{A|x} \otimes M_{B|y}) \left(\sum_i p_i \hat{\rho}_A^{(i)} \otimes \hat{\rho}_B^{(i)}\right)\right] \\ &= \sum_i p_i \underbrace{\text{Tr}(M_{A|x} \hat{\rho}_A^{(i)})}_{p(a|x, \lambda)} \cdot \underbrace{\text{Tr}(M_{B|y} \hat{\rho}_B^{(i)})}_{p(b|y, \lambda)} \\ &= \sum_i p_i p(a|x, \lambda) p(b|y, \lambda) \end{aligned} \quad (3.25)$$

and thereby satisfy the locality condition 3.13. So every separable state admits a local hidden variable model. Interestingly the converse is not true. Just because a state admits a local hidden variable model, it doesn't have to be separable. For instance, the Werner state

$$\rho_W = p |\phi^+\rangle\langle\phi^+| + \frac{1}{4}(1-p)\mathbb{1} \quad (3.26)$$

is separable only for $p \leq \frac{1}{3}$ but allows an LHV model up to $p = 0.66$ [AGT06].⁴ This means that entanglement does not imply nonlocality. But what does? One longstanding guess was ventured by Asher Peres in 1998.

It is plausible that quantum systems whose density matrix has a positive partial transposition satisfy all these inequalities [the Bell inequalities], and therefore are compatible with local objective variables, even if their quantum properties are essentially nonlocal. [Per98]

Put shortly, he conjectures that if an entangled state has a positive partial transpose, it admits a local hidden variable model. Quite often the Peres conjecture is mentioned in the context of *bound entangled* states.

⁴See [BCP⁺14, p.21] for an explicit LHV model for $p = \frac{1}{2}$.

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Bound entanglement

So far we have only considered the pure entangled state $|\phi^+\rangle$. This state is *maximally entangled*, which means that each of the subsystems is in a perfectly mixed state, that we cannot obtain any information about one of the subsystems alone. A paradigmatic example for maximally entangled states for the CHSH-case are the so-called *Bell states*:

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \quad |\phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \quad (3.27)$$

$$|\psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \quad |\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \quad (3.28)$$

Now let's suppose Alice and Bob share an arbitrary ensemble of entangled states ρ . Then each of them can perform local operations on his/her particles, thereby changing the state of the system. They can also exchange classical information, such as texting each other, which operation they performed. These actions are summarised in the term *LOCC*: local operations and classical communication. Sometimes they can produce one or more pairs of maximally entangled particles through LOCC. In this case they have *distilled* maximally entangled states from ρ . However, not every ensemble can be distilled. Ensembles, which cannot be distilled are called *bound entangled*.

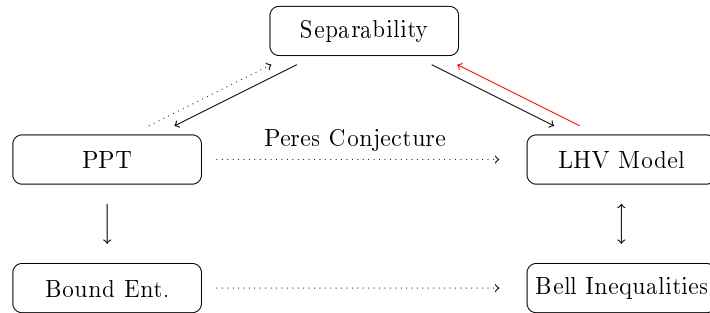


Figure 3.5.: Relations between separability, the existence of local hidden variable models, bound entanglement, Bell's inequalities and the positivity of the partial transpose. The dashed lines indicate that the relations only hold for certain scenarios while the red line indicates that the admittance of an LHV-model does *not* imply separability.

Now we are in a position to draw a connection between bound entangled states and the Peres conjecture. In their 1998 paper [HHH98] the Horodeckis showed that PPT implies bound entanglement. To do so, they first proved that any LOCC-action preserves the positivity of the partial transpose. Then they assumed that there exists a PPT state ρ that can be distilled. This means that one can obtain a 2×2 maximally entangled state via LOCC from ρ . Because the LOCC-action does not change the positivity of the partial transpose, this state must be a PPT-state as well. But for systems with dimension 2×2

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the PPT-criterion is sufficient for separability. Therefore the maximally entangled state has to be separable, which is clearly a contradiction.

As PPT implies bound entanglement, one can formulate a stronger version of the Peres conjecture by restricting it to bound entangled states. However, even in this restricted version, the conjecture was disproved by Vértesi and Brunner, who found an undistillable state violating a Bell inequality.⁵ Yet this state was only found numerically and does not provide any further insight into the connection between PPT-states and local models. To obtain a deeper understanding of this connection we will introduce a new method that allows us to study the Peres conjecture more closely for a given Bell scenario and apply it to the particular case of $(3, 2, 2)$.

⁵See [VB12] for the multipartite case ($n > 2$) and [VB14] for the bipartite case ($n = 2$).

4. The Local Polytope

As mentioned before, the CHSH inequality is just one of many Bell inequalities, each corresponding to a particular scenario (n,m,d) . In this section we will discuss how to generate the Bell inequalities for a given scenario, using a fascinating connection to convex polytopes. To do so, we first need to lay the theoretical foundations, which is why in Section 4.1 we will be discussing the relevant definitions and theorems from the field of convex polytopes. Building on this, we will construct the so-called local polytope and present an algorithm to generate a minimal set of Bell inequalities constraining it.

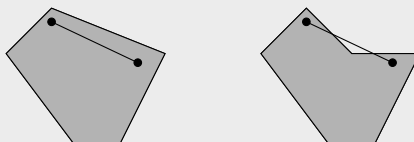
4.1. Convex Polytopes

4.1.1. Definitions

Definition 8. A point set $K \subseteq \mathbb{R}^s$ is convex if for any two points $x_1, x_2 \in K$ it also contains the straight line segment

$$[x_1, x_2] = \{\lambda x_1 + (1 - \lambda)x_2 | 0 \leq \lambda \leq 1\}^1 \quad (4.1)$$

For example, in the figures below, the set on the left is convex, while the set on the right is not.



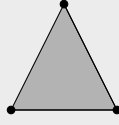
Definition 9. For any $K \subseteq \mathbb{R}^d$ the convex hull $\text{conv}(K)$ is the smallest convex set containing K :

$$\text{conv}(K) \equiv \cap \{K' \subseteq \mathbb{R}^d : K \subseteq K', K' \text{ convex}\} \quad (4.2)$$

For example, the convex hull of the three points in general position in 2D is the triangle obtained by connecting each of the points with a straight line plus its interior.

¹This definition and the following definitions in this subsection are taken from [Zie07, p.3-4, 28-29].

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The convex hull of a given set K is equivalent to the set of all convex combinations of points x_i in K :

$$\text{conv}(K) = \left\{ \sum_{i=1}^n \lambda_i x_i \mid n \in \mathbb{N}, x_i \in K, \lambda_i \geq 0, \sum_{i=1}^n \lambda_i = 1 \right\} \quad (4.3)$$

This can be seen as follows: Each convex set containing K must, by definition 8, contain all convex combinations of points in K , so the set of all convex combinations is a subset of $\text{conv}(K)$. Conversely, the set of all combinations of points in K is itself a convex set containing K , which is why the two sets must be equal.

Definition 10. A \mathcal{V} -polytope² is the convex hull of a finite set of points in \mathbb{R}^d .

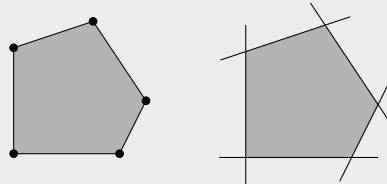
$$\mathcal{P}_{\mathcal{V}} = \text{conv}(V) \text{ for some } V \in \mathbb{R}^{d \times n} \quad (4.4)$$

An \mathcal{H} -polytope is a bounded intersection of finitely many closed halfspaces in \mathbb{R}^d .

$$\mathcal{P}_{\mathcal{H}} = P(A, z) = \{x \mid Ax \leq z\} \text{ for some } A \in \mathbb{R}^{d \times m}, z \in \mathbb{R}^m \quad (4.5)$$

A polytope is a point set $\mathcal{P} \subseteq \mathbb{R}^d$ that can be represented as a \mathcal{V} - or as an \mathcal{H} -Polytope.³

The figures below illustrate the difference between a \mathcal{V} -polytope (left) and an \mathcal{H} -polytope (right).



Before moving on to the dimension of polytopes, we first need to introduce the concepts of the affine subspace [Fis00, p.116] and affine hull [Zie07, p.3].

²As only convex polytopes are of relevance in this thesis, we will simply call them “polytopes” in the following.

³We will soon see that each \mathcal{V} -polytope admits a description as an \mathcal{H} -polytope and vice versa.

4. The Local Polytope

Definition 11. If V is a vector space, then $X \subseteq V$ is called an affine subspace if $X = \emptyset$ or if there is a $v \in V$ and a subspace $W \subset V$ such that

$$X = v + W = \{u \in V \mid \exists w \in W : u = v + w\} \quad (4.6)$$

If $X \neq \emptyset$, the dimension of X is equal to the dimension of W . Any affine subspace can be represented as the affine hull of a finite point set. The affine hull of a point set S is the smallest affine subspace containing S :

$$\text{aff}(S) = \left\{ \sum_{i=1}^k \lambda_i x_i \mid k > 0, x_i \in S, \lambda_i \in \mathbb{R}, \sum_{i=1}^k \lambda_i = 1 \right\} \quad (4.7)$$

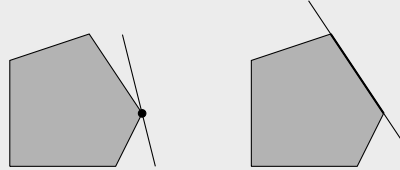
Definition 12. The dimension of a polytope is the dimension of its affine hull. A polytope of dimension d is called a d -polytope.

Definition 13. Let $\mathcal{P} \subseteq \mathbb{R}^n$ be a convex polytope. A set of the form

$$F = \mathcal{P} \cap \{x \in \mathbb{R}^d : c^T x = c_0\} \quad (4.8)$$

where $c^T x \leq c_0$ is satisfied for all points $x \in \mathcal{P}$ is called a face of \mathcal{P} . Faces of dimension 0, 1 and $(\dim(\mathcal{P}) - 1)$ are called vertices, edges and facets, respectively.

The figures below show the inequality $c^T x \leq c_0$ for a vertex (left) and a facet (right) of a 2-polytope.



4.1.2. The Representation Theorem

The main theorem for convex polytopes is the following:

Theorem 1. A subset $\mathcal{P} \subseteq \mathbb{R}^d$ is a \mathcal{V} -polytope if and only if it is an \mathcal{H} -polytope.

This is quite a remarkable result - it allows us to choose between the vertex- and the half-space-representation for any polytope. We will not prove the theorem rigorously but provide a sketch for the direction $\mathcal{V} \rightarrow \mathcal{H}$ which will be of great importance when it comes to generating Bell inequalities.⁴ This proof relies on an algorithm called the Fourier-Motzkin elimination (FME).

⁴For a complete proof see, for example, [Zie07].

4. The Local Polytope

Fourier-Motzkin elimination

The Fourier-Motzkin elimination is similar to gaussian elimination [MG07]. While gaussian elimination is used to find solutions for a system of linear equations, FME is used to reduce the number of variables in a system of linear inequalities. The algorithm is based on the idea that a one-dimensional system of linear inequalities

$$\begin{aligned} x \geq p_1, \dots, x \geq p_n & \Leftrightarrow x \geq p_1, \dots, x \geq p_n \\ x \leq q_1, \dots, x \leq q_m & \Leftrightarrow -x \geq -q_1, \dots, -x \geq -q_m \end{aligned}$$

only holds if $\forall i = 1, \dots, n, j = 1, \dots, m : q_j \geq p_i$. This allows us to eliminate x by adding the inequalities on the right pairwise. In general, given an n -dimensional set of inequalities indexed by (i) :

$$a_{i1}x_1 + \dots + a_{in}x_n \geq b_i \quad (i) \quad (4.9)$$

with variables $x_1, \dots, x_n, i = 1, \dots, m$ and $a_{ij} \in \mathbb{R}$, we can gradually eliminate all the x_k s by iterating the following steps:

- $\forall i : a_{ik} \neq 0$ multiply inequality (i) by $\frac{1}{|a_{ik}|}$
- $\forall i : a_{ik} = 0$ copy inequality (i) .
- For any pair of $a_{ik} > 0$ and $a_{i'k} < 0$ add the inequalities (i) and (i') to obtain a new inequality that is independent of x_k .

By repeating these steps m times, one obtains a set of inequalities that is independent of any x_1, \dots, x_m .

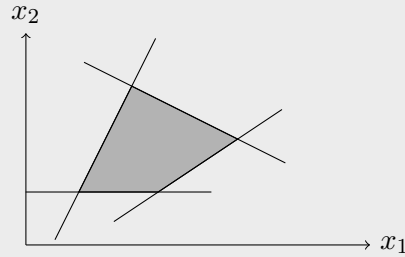
Consider the polytope defined by the following equations:

$$-2x_1 + 3x_2 \geq -2 \quad (1)$$

$$-x_1 - 2x_2 \geq -8 \quad (2)$$

$$2x_1 - x_2 \geq 1 \quad (3)$$

$$x_2 \geq 1 \quad (4)$$



Our goal is to eliminate x_2 . To do so, we read off the coefficients for x_2 ($a_{12} = 3$, $a_{22} = -2$, $a_{32} = -1$, $a_{42} = 1$) and multiply each of the inequalities with $\frac{1}{|a_{i2}|}$.

$$-\frac{2}{3}x_1 + x_2 \geq -\frac{2}{3} \quad (1)$$

$$-\frac{1}{2}x_1 - x_2 \geq -4 \quad (2)$$

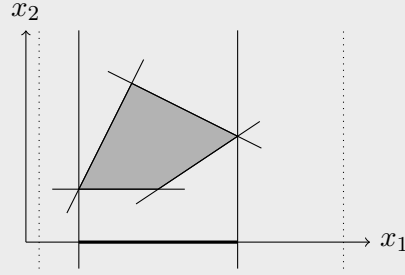
$$2x_1 - x_2 \geq 1 \quad (3)$$

$$x_2 \geq 1 \quad (4)$$

4. The Local Polytope

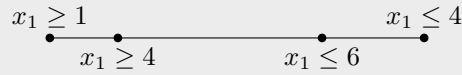
Then we add the inequalities with differing signs in front of x_2 and simplify.

$$\begin{aligned} (1) + (2) : x_1 &\leq 4 \\ (1) + (3) : x_1 &\geq \frac{1}{4} \\ (2) + (4) : x_1 &\leq 6 \\ (3) + (4) : x_1 &\geq 1 \end{aligned}$$



We have thereby successfully eliminated x_2 . One can, however, see that the two equations in the middle are redundant. Removing them yields $1 \leq x_1 \leq 4$. The line defined by these two inequalities is the projection onto $x_2 = 0$.

The redundant inequalities can also be identified by constructing the *dual polytope*. This is the polytope one obtains by representing each inequality with a point.⁵In the case of our projected polytope we would obtain a line segment defined by four points:



The extreme points of the dual polytope correspond to the non-redundant inequalities.

We can now use this method to construct the corresponding half-space-representation to any \mathcal{V} -polytope

$$\mathcal{P} = \text{conv}(V). \tag{4.10}$$

By the definition of the convex hull 4.3, x is an element of \mathcal{P} iff for $v_1, \dots, v_n \in V$

$$\exists \lambda_1, \dots, \lambda_n \geq 0 \tag{4.11}$$

$$\text{such that } \lambda_1 + \dots + \lambda_n = 1 \tag{4.12}$$

$$\lambda_1 v_1 + \dots + \lambda_n v_n = \mathbf{x} \tag{4.13}$$

By rewriting each equality $a = b$ as $a \geq b$ and $-a \geq -b$, we obtain a set of inequalities depending on the coefficients λ_i and x . Using the Fourier-Motzkin algorithm, we can gradually eliminate every λ_i and thereby obtain a set of linear inequalities involving only the elements of the vector \mathbf{x} . These inequalities fully characterise the elements of \mathcal{P} . By arranging them in a matrix inequality $A\mathbf{x} \geq \mathbf{z}$ we can represent the polytope as

$$\mathcal{P} = \{\mathbf{x} | A\mathbf{x} \geq \mathbf{z}\}, \tag{4.14}$$

⁵For the construction of the dual polytope see [Zie07, p.61].

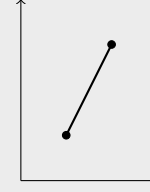
4. The Local Polytope

which is an \mathcal{H} -polytope by construction.

Take, for example, the 1-polytope⁶

$$\mathcal{P} = \text{conv} \left(\left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 3 \end{pmatrix} \right\} \right). \quad (4.15)$$

This corresponds to a line in \mathbb{R}^2 , represented in the figure on the right. The convex hull is in this case defined by



$$\begin{aligned} \lambda_1 + \lambda_2 &= 1 & \lambda_1 &\geq 0 \\ \lambda_1 + 2\lambda_2 &= x_1 & \lambda_2 &\geq 0 \\ \lambda_1 + 3\lambda_2 &= x_2 \end{aligned}$$

One could now rewrite this as a set of linear inequalities and use the Fourier-Motzkin algorithm to eliminate λ_1 and λ_2 . However, in this case, there is an easier way to eliminate the coefficients. In the first step we set $\lambda_1 = 1 - \lambda_2$ and obtain

$$\begin{aligned} \lambda_2 &= x_1 - 1 & -\lambda_2 &\geq -1 \\ 2\lambda_2 &= x_2 - 1 & \lambda_2 &\geq 0 \end{aligned}$$

Inserting $\lambda_2 = x_1 - 1$ into the other equations and simplifying gives

$$2x_1 - x_2 = 1 \qquad -x_1 \geq -2 \qquad x_1 \geq 1$$

By rewriting the equation as two inequalities, we are left with a set of four linear inequalities depending only on x_1 and x_2 . These are represented by the following matrix inequality:

$$A\mathbf{x} \equiv \begin{pmatrix} 2 & -1 \\ -2 & 1 \\ -1 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \geq \begin{pmatrix} 1 \\ -1 \\ -2 \\ 1 \end{pmatrix} \equiv \mathbf{z}$$

One should keep in mind that the Fourier-Motzkin algorithm produces a lot of redundant inequalities, because it simply adds any pair of inequalities whose coefficients differ in sign. It therefore makes sense to check each of the newly generated sets of inequalities for

⁶This example is based on [Mat15].

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redundancies and remove the unnecessary ones. One can identify a redundant inequality by checking if it is trivially satisfied when all of the other inequalities hold [GGP16]. To do so we define

- $A^{(i)}$: the matrix obtained by removing the i -th row of A
- $\mathbf{b}^{(i)}$: the vector obtained by removing the i -th entry of \mathbf{b}
- \mathbf{a}_i^T : the i -th row of A
- b_i : the i -th entry of \mathbf{b}

and then calculate

$$b^* = \min_{\mathbf{x}: A^{(i)}\mathbf{x} \geq \mathbf{b}^{(i)}} \mathbf{a}_i^T \mathbf{x} \quad (4.16)$$

If $b^* \geq b_i$, then $\mathbf{a}_i^T \mathbf{x} \geq b_i$ for all \mathbf{x} satisfying the other inequalities, so the i -th inequality must be redundant.

4.2. Locality Constraints

Now it is time to build the connection from convex polytopes to Bell inequalities [TAS⁺15, WW01]. Recall that in general the Bell inequalities correspond to a given scenario with n parties, m measurements and d outcomes. Labelling the i -th party's choice of measurement with $x_i \in \{0, \dots, m-1\}$ and the corresponding outcome with $a_i \in \{0, \dots, d-1\}$ we can describe each scenario with the probabilities

$$p(a_0, \dots, a_{n-1} | x_0, \dots, x_{n-1}) \equiv p(\mathbf{a} | \mathbf{x}) \quad (4.17)$$

As there are m^n possible combinations of measurements, each with d^n possible outcomes, there are $(md)^n$ such probabilities. These probabilities can be arranged in a vector \mathbf{P} lying in a space of dimension $(md)^n$. This space is constrained by the non-negativity of the probabilities

$$\forall \mathbf{a}, \mathbf{x} : p(\mathbf{a} | \mathbf{x}) \geq 0 \quad (4.18)$$

and the normalisation constraints for each choice of measurements

$$\forall \mathbf{x} \sum_{a_0, \dots, a_{n-1}} p(a_0, \dots, a_{n-1} | \mathbf{x}) = 1. \quad (4.19)$$

The above (in)equalities define a polytope \mathcal{P} of dimension $m^n(d^n - 1)$.

4. The Local Polytope

For the CHSH-case we have $n = 2$ parties, $m = 2$ measurements $x_0 \in \{0, 1\}$ and $x_1 \in \{0, 1\}$ and $d = 2$ outcomes $a_0 \in \{-1, 1\}$ and $a_1 \in \{-1, 1\}$. Therefore one can assign $(2 \cdot 2)^2 = 16$ probabilities $p(a_0, a_1 | x_0, x_1)$ to the Bell scenario. There are four normalisation constraints like

$$p(1, 1|0, 0) + p(1, -1|0, 0) + p(-1, 1|0, 0) + p(-1, -1|0, 0) = 1, \quad (4.20)$$

so only 12 probabilities remain independent from each other.

No-signalling constraints

However, some of the probability-vectors in \mathcal{P} are not physical because they violate the *no-signalling principle*. According to this principle it is impossible to transmit signals instantaneously. To exclude these un-physical vectors from our polytope, we have to impose additional constraints. In mathematical terms, the *no-signalling principle* can be formulated as follows [BCP⁺14, TAS⁺15]:

$$\sum_{a_i} p(\mathbf{a} | x_0, \dots, x_i, \dots, x_{n-1}) = \sum_{a_i} p(\mathbf{a} | x_0, \dots, x'_i, \dots, x_{n-1}) \quad \forall x'_i \neq x_i \quad (4.21)$$

This means that the choice of measurement of one party does not influence the statistics observed by the other parties. The no-signalling constraints reduce the dimension of the polytope to $[(d-1)m+1]^n - 1$.⁷ We denote the new polytope by \mathcal{P}_{NS} .

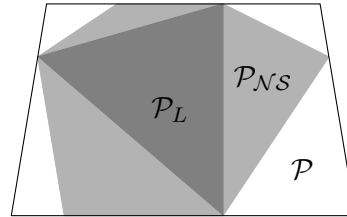
Locality constraints

Finally we want to restrict our description to probabilities that can be described by LHV models. These probabilities have to satisfy the generalised version of equation 3.13:

$$p(\mathbf{a} | \mathbf{x}) = \int_{\Lambda} d\lambda q(\lambda) \prod_{i=0}^{n-1} p(a_i | x_i, \lambda) \quad (4.22)$$

By imposing the condition above, we reduce the allowed region in space to a new polytope, which we will call the *local polytope* and denote by \mathcal{P}_L . It is a subset of the no-signalling polytope and has the same dimension [TAS⁺15, p.4].

The different polytopes are represented in the figure on the right. An important feature of the vectors within the local polytope is that they can be expressed as a convex combination of deterministic events [Fin82].



In a deterministic event the outcomes are known completely, so the corresponding probabilities are either zero or one. We can describe them with delta functions $\delta(a_i, f(x_i, \lambda))$

⁷See appendix B.

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where $f(x_i, \lambda)$ produces an outcome in $\{0, \dots, d-1\}$ based on the information available to the i -th party, namely x_i and λ . If $f(x_i, \lambda) = a_i$, the probability of obtaining outcome a_i is one, otherwise it is zero. If the outcomes are not known completely, we can describe the system of the i -th party by assigning probabilities p_{j_i} to each possible outcome:

$$p(a_i|x_i, \lambda) = \sum_{j_i} p_{j_i} \delta(a_i, f_{j_i}(x_i, \lambda)) \quad (4.23)$$

Inserting this into the locality condition we obtain

$$p(\mathbf{a}|\mathbf{x}) = \sum_{j_0, \dots, j_{n-1}} p_{j_0} \cdot \dots \cdot p_{j_{n-1}} \int d\lambda \rho(\lambda) \prod_{i=0}^{n-1} \delta(a_i, f_{j_i}(x_i, \lambda)) \quad (4.24)$$

$$= \int d\lambda \tilde{\rho}(\lambda) \prod_{i=0}^{n-1} \delta(a_i, f_{j_i}(x_i, \lambda)), \quad (4.25)$$

by merging sum and integral into a new probability distribution $\tilde{\rho}(\lambda)$. Equation 4.25 tells us that each vector inside the local polytope can be represented as a convex combination of local deterministic points

$$\mathbf{p}^{(d)} = \prod_{i=0}^{n-1} \delta(a_i, f_{j_i}(x_i, \lambda)) \in \{0, 1\}, \quad (4.26)$$

which implies that the local polytope is the convex hull of these points, i.e.

$$\mathcal{P}_L = \text{conv}(\{\mathbf{p}^{(d)}\}). \quad (4.27)$$

As $\{0, 1\}$ are the extremal values for probabilities, the points $\mathbf{p}^{(d)}$ correspond to the extreme points of the local polytope. This is a particularly useful result as we now only need to know a finite set of points to describe the local polytope. Furthermore, it is rather easy to generate $\{\mathbf{p}^{(d)}\}$: One simply assigns a fixed value to each outcome and calculates the corresponding probabilities. For an (n, m, d) scenario there are $d^{(nm)}$ possible assignments and thereby local deterministic points.

As an example, we generate a deterministic vector $\mathbf{p}^{(d)}$ of the $(2, 2, 2)$ -polytope, corresponding to the outcomes $a_0 = a_1 = b_0 = +1$ and $b_1 = -1$. In this case

$$p(+1 + 1|00) = p(+1 + 1|10) = p(+1 - 1|01) = p(+1 - 1|11) = 1 \quad (4.28)$$

while all other probabilities are zero. $\mathbf{p}^{(d)}$ is obtained by combining all these probabilities in a vector of dimension $[(d-1)m + 1]^n - 1 = 8$.

Once we know the vertices defining the polytope, we can use Fourier-Motzkin elimination to generate the constraining inequalities - the Bell inequalities.

4. The Local Polytope

4.2.1. Correlator-Description

As the Bell inequalities are sometimes written in terms of correlators (expectation values), just like the CHSH-inequality 3.18, we need to find a way to go from probabilities $p_{ia_i} \equiv p(a_i)$ to correlators

$$\langle A_x^{(i)} \rangle_k = \sum_i p_{ia_i} a_i^k \quad (4.29)$$

where i denotes the party, x the choice of measurement and k the order of the correlator. To express the probabilities in terms of correlators, we make use of the *discrete Fourier transform* (DFT) [Fra13, p.178 ff.]. The DFT converts a sequence of complex numbers

$$f_k = \sum_{j=0}^{N-1} \hat{f}_j e^{\frac{2\pi i}{N} jk} \quad (4.30)$$

into another sequence of complex numbers

$$\hat{f}_j = \frac{1}{N} \sum_{k=0}^{N-1} f_k e^{\frac{2\pi i}{N} jk}. \quad (4.31)$$

To apply the discrete Fourier transform to our problem, we need to express the outcomes in terms of primitive roots of unity: $a_i \in \{\exp(\frac{2\pi i}{d} j)\}$ where j ranges from 0 to $d-1$.

For example, for $d=2$ we can rewrite the outcomes as

$$1 = \exp(i\pi \cdot 0), \quad -1 = \exp(i\pi \cdot 1).$$

This way, the correlators take the form

$$\langle A_x^{(i)} \rangle_k = \sum_{j=0}^{d-1} e^{\frac{2\pi i}{d} jk} p_{ij} \quad (4.32)$$

Due to the locality constraint the correlators satisfy $\langle A_i^k A_j^l \rangle = \langle A_i^k \rangle \langle A_j^l \rangle$ for $i \neq j$ on the vertices. Therefore

$$\langle A_{i_1} \cdots A_{i_n} \rangle_{k_1, \dots, k_n} = \sum_{j_1, \dots, j_n=0}^{d-1} p_{i_1 j_1} \cdots p_{i_n j_n} e^{\frac{2\pi i}{d} j_1 k_1} \cdots e^{\frac{2\pi i}{d} j_n k_n} \quad (4.33)$$

With the multi-dimensional version of the discrete Fourier transform we can convert this into

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$$p_{i_1 j_1} \dots p_{i_n j_n} = \frac{1}{(d-1)^n} \sum_{k_1, \dots, k_n=0}^{d-1} \langle A_{i_1} \dots A_{i_n} \rangle_{k_1, \dots, k_n} e^{-\frac{2\pi i}{d} j_1 k_1} \dots e^{-\frac{2\pi i}{d} j_n k_n} \quad (4.34)$$

The formula above allows us to rewrite any probabilities in terms of correlators. In general one has to use imaginary outcomes to rewrite them in terms of primitive roots of unity. In the following we will, however, focus on the $d = 2$ case with the real outcomes 1 and -1 .

5. Classes of Bell Inequalities

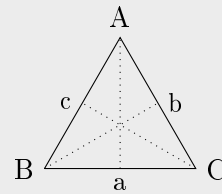
Now we know everything we need to generate the Bell Inequalities. Usually the number of inequalities is incredibly high, though. For the $(3, 2, 2)$ case, for example, there are 53856 inequalities [PS01]. These inequalities, however, can be grouped into *classes*, i.e. orbits with respect to certain symmetry groups.¹

Definition 14. Given a group $G \curvearrowright X$, the orbit of an element $x \in X$ is given by the set of elements into which x can be transformed by the elements of G [Mei08].

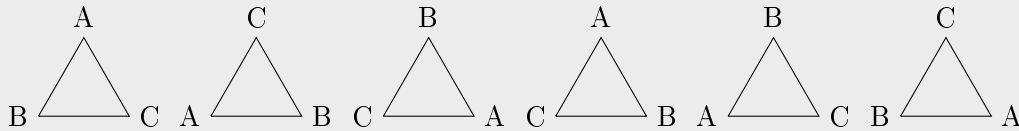
$$\text{Orb}(x) = \{g \cdot x | g \in G\} \tag{5.1}$$

One example for symmetry groups are transformations of the equilateral triangle that project every edge onto another edge. The possible symmetry transformations are:

- clockwise rotation by 120°
- anti-clockwise rotation by 120°
- reflection through the axes a , b and c
- trivial transformation (identity)



Applying these transformations to the triangle on right gives out six different triangles.



The set of these triangles is the orbit of the triangle ABC with respect to the symmetry group containing the transformations above.

¹Recall that a *group* is a set G with elements g and an operation \circ combining the elements such that

1. $g_1, g_2 \in G \Rightarrow g_1 \circ g_2 \in G$
2. \exists an element 1 such that $\forall g \in G : 1 \circ g = g \circ 1 = g$
3. $\forall g \in G \exists g^{-1} \in G : g^{-1} \circ g = g \circ g^{-1} = 1$
4. $g_1 \circ (g_2 \circ g_3) = (g_1 \circ g_2) \circ g_3$

Furthermore, an *action* of a group G on a set X , denoted $G \curvearrowright X$, is a map from $G \times X \rightarrow X$ such that [Mei08]

1. $\forall x \in X : 1 \cdot x = x$
2. $\forall g_1, g_2 \in G$ and $x \in X : (g_1 g_2) \cdot x = g_1 \cdot (g_2 \cdot x)$

5. Classes of Bell Inequalities

In a scenario (n, m, d) where all parties can choose between the same number of measurement apparatuses with the same number of outcomes, the naming of parties, observables or outcomes does not make a physical difference. Therefore the permutations of elements corresponding to

- renaming parties
- renaming the observables of one party
- renaming the outcomes of one observable

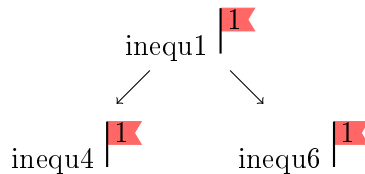
generate a symmetry group. The Bell inequalities belonging to the same orbit with respect to this symmetry group do not differ in a physically relevant sense. It therefore suffices to analyse one Bell inequality to obtain results that are valid for all the inequalities in its orbit. This feature will prove to be very useful in Chapter 7, in which we analyse a set of over 5000 Bell inequalities. Generating all elements of the symmetry group and sorting a large set of Bell inequalities into orbits can, however, be quite complicated [RBG14]. A useful algorithm, allowing us to group the Bell inequalities without explicitly generating all elements of the symmetry group, is the *breadth-first search algorithm*.

5.1. Breadth-First Search

The breadth-first search algorithm [Cor09, Top17] is used to explore graphs. A graph is an abstract data type, consisting of points (*nodes*) and their connections (*edges*). We'll call the nodes that are connected via an edge "neighbours". In our case, the nodes are the Bell inequalities and the edges represent symmetry transformations. In the beginning, however, we do not know the connections. All we have is a list of all the Bell inequalities generated by FME:

- inequ1
- inequ2
- inequ3
- ⋮

The BFS algorithm now takes the first inequality, assigns it to class 1 and performs all of the generating symmetry transformations on it to obtain its direct neighbours.

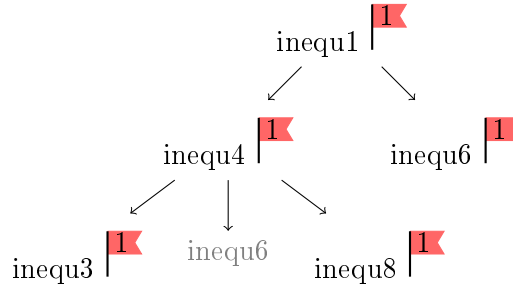


5. Classes of Bell Inequalities

It then flags all the generated inequalities as belonging to the same class as `inequ1` and adds them to a queue.

`q:inequ4, inequ6`

In the next step it takes the first inequality waiting in line, removes it from the queue and generates all of its neighbours.



To avoid getting stuck in an infinite loop, the algorithm first checks whether the inequality has already been flagged (such as `inequ6`) before proceeding. It then flags the remaining inequalities and adds them to the queue as well.

`q:inequ6, inequ3, inequ8`

Notice that the next inequality in line is `inequ6`. This is the key feature of the BFS algorithm: Instead of following down one path as far as possible before backtracking², it adds the newly generated elements to the end of the queue and first analyses all of the direct neighbours. Continuing in the same way as illustrated above until all of the newly generated neighbours have already been flagged, it finds all of the elements in the orbit of `inequ1`. Then it takes the next unflagged inequality, marks it as belonging to class 2 and starts anew. This continues until all inequalities have been assigned a class. As it is quite easy to implement a symmetry that only exchanges one party, renames measurements or changes outcomes, the BFS algorithm is straightforward for our problem. We will see an example of classes of Bell inequalities generated via BFS in Chapter 7.

²This is called depth-first search.

6. A Method to Generate PPT Bounds

In this chapter we present a novel method to derive bounds on the minimal value achievable for any PPT-states $|\psi\rangle \in \mathcal{H}$ on a given Bell inequality – the so-called *PPT-bounds*. This will lay the groundwork for the following chapter, in which we use this method to compute the PPT-bounds for a certain set of inequalities for the Bell scenario (3, 2, 2).

The method is based on two concepts, which we will introduce in the subsequent two sections: semidefinite programming (SDP) and the sum-of-squares-decomposition of a given polynomial. The former will provide us with the necessary tools to find a bound on the minimal value that a given Bell inequality $\langle B \rangle - \beta \geq 0$ ¹ can take over all possible quantum states (*quantum bound*) and PPT-states (*PPT-bound*) respectively. The results of the SDP-programme together with the theoretical framework developed in Section 6.2 will additionally provide an analytical proof that the obtained quantum/PPT-bound is valid indeed.

6.1. Semidefinite Programming

A semidefinite programming (SDP) problem is a convex optimisation problem.² The goal is to minimise or maximise a linear function while making sure that it satisfies a number of constraints in the form of linear matrix inequalities

$$A_0 + \sum_i A_i x_i \succeq 0 \tag{6.1}$$

where $A_i \in \mathcal{S}^n$ are real, symmetric matrices. An SDP problem can be expressed in one of the following two canonical forms

<p>primal problem minimise $\langle C, X \rangle = \text{Tr}(C^T X)$ subject to $\langle A_i, X \rangle = b_i, X \succeq 0$</p>	<p>dual problem maximise $\mathbf{b}^T \mathbf{y}$ subject to $\sum_{i=1}^m A_i y_i \preceq C$</p>
--	---

where $C, A_i \in \mathcal{S}^n$. To understand the relationship between the primal and the dual problem, it is helpful to consider an example. The following example [Wik17] considers a special case of semidefinite programming, namely *linear programming*, where the matrices C and X are both diagonal. In this case, the function to be minimised can be rewritten as $\text{Tr}(C^T X) = \mathbf{c}^T \mathbf{x}$ where \mathbf{c} and \mathbf{x} are vectors of the diagonal elements of C and X respectively.

¹In the following we will refer to B as *Bell operator* and as classical bound to β . In the CHSH-case the Bell operator is $(-A_0 B_0 - A_0 B_1 - A_1 B_0 + A_1 B_1)$ while the classical bound is -2 .

²This section follows the presentation in [BPT13, chapter 2].

6. A Method to Generate PPT Bounds

A farmer produces two kinds of crops: x_1 and x_2 . To grow each of the crops he needs a certain amount of fertiliser y_1 and pesticide y_2 : Two units of fertiliser and one unit of pesticide for x_1 and one unit each for x_2 . All together he has eight units of fertiliser and six units of pesticide at his disposal. The optimisation problem the farmer has to solve is the following:

“How can I maximise the profit, if I can sell crop x_1 for 3€ and crop x_2 for 2€?”

Formally, this problem can be written as

$$\begin{array}{ll}
 \text{maximise: } p = 3x_1 + 2x_2 & \text{maximize: } p = \mathbf{c}^T \mathbf{x} \\
 \text{subject to: } 2x_1 + x_2 \geq 8 & \text{subject to: } A\mathbf{x} \geq \mathbf{b} \\
 x_1 + x_2 \geq 6 & \mathbf{x} \geq \mathbf{0} \\
 x_1, x_2 \geq 0 &
 \end{array}$$

where the last inequality just expresses the fact that the farmer produces a non-zero amount of crops. This *primal problem* can also be expressed in the matrix form on the right by defining

$$\mathbf{c} = \begin{pmatrix} 3 \\ 2 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}, \quad \mathbf{b} = (8 \ 6).$$

Now let's assume that someone wants to buy fertiliser and pesticide from the farmer. Of course the farmer will not sell his products unless he makes at least the same profit selling the fertiliser and pesticide as he would, if he'd raise and sell the crops. So the buyer has to solve the problem

“How can I minimise the costs while making sure that the farmer makes at least the same amount of money?”

In mathematical terms:

$$\begin{array}{ll}
 \text{minimise: } m = 8y_1 + 6y_2 & \text{minimise: } m = \mathbf{b}^T \mathbf{y} \\
 \text{subject to: } 2y_1 + y_2 \geq 3 & \text{subject to: } A^T \mathbf{y} \geq \mathbf{c} \\
 y_1 + y_2 \geq 2 & \mathbf{y} \geq \mathbf{0} \\
 y_1, y_2 \geq 0 &
 \end{array}$$

where $\mathbf{y} = (y_1, y_2)^T$. This is the *dual problem*.

There is an interesting relation between the primal and the dual problem, known as *weak duality*, which can be obtained by considering the following term:

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$$\langle C, X \rangle - \mathbf{b}^T \mathbf{y} = \langle C, X \rangle - \sum_{i=1}^m y_i \langle A_i, X \rangle = \langle C - \sum_{i=1}^m A_i y_i, X \rangle \geq 0 \quad (6.2)$$

Equation 6.2 tells us that the value of the primal function at X is always greater than or equal to the value of the dual function at any \mathbf{y} and thereby provides a lower bound for $\langle C, X \rangle$ and an upper bound for $\mathbf{b}^T \mathbf{y}$. Furthermore, it allows us to see whether there exist primal and dual *optimal solutions*, that is solutions that minimise $\langle C, X \rangle$ and maximise $\mathbf{b}^T \mathbf{y}$ respectively. Using that $\langle X, Y \rangle = 0$ iff $XY = YX = 0$ for $X, Y \succeq 0$ one can see that (X, \mathbf{y}) are primal and dual optimal solutions if and only if

$$(C - \sum_{i=1}^m A_i y_i)X = 0 \quad (6.3)$$

Finally, one should remark that it is possible to choose $C = 0$. In this case, there is no function to maximise/minimise and the problem is called *feasibility problem*. The goal of such a feasibility problem is simply to determine if there exists a matrix X satisfying the constraints.

6.2. Sums of Squares

Before we apply our method to Bell inequalities, we will take a closer look at the sum of squares (sos) decomposition of polynomials.³

Definition 15. *A polynomial of n variables and degree $2d$, $p(x) \in \mathbb{R}\mathbf{x}_{2d}$, is a sum of squares if there exist $q_1, \dots, q_m \in \mathbb{R}\mathbf{x}_d$ such that*

$$p(x) = p_{2d}x^{2d} + p_{2d-1}x^{2d-1} + \dots + p_1x + p_0 = \sum_{k=1}^m q_k^2(x) \quad (6.4)$$

Because each of the terms in the sum is non-negative, it immediately follows that if $p(x)$ is a sum of squares it is also non-negative. The converse, however, is only true for univariate polynomials ($n = 1$), quadratic polynomials ($2d = 2$) and bivariate quartics ($n = 2$, $2d = 4$) [BPT13, p.59]. In general there exist non-negative polynomials that cannot be written as sums of squares. One example is the Motzkin-polynomial [BPT13, p.59]:

$$M(x, y) = x^4y^2 + x^2y^4 + 1 - 3x^2y^2. \quad (6.5)$$

However, there is a criterion both necessary and sufficient for $p(x)$ being a sum of squares. We will start by looking at the criterion for univariate polynomials and then generalise it to the multivariate case.

³This section follows the presentation in [BPT13, chapter 3].

6.2.1. Univariate Polynomials

Let $p(x)$ be a univariate polynomial of degree $2d$:

$$p(x) = p_{2d}x^{2d} + p_{2d-1}x^{2d-1} + \cdots + p_1x + p_0 \quad (6.6)$$

If it is a sum of squares, then there exist q_1, \dots, q_m of degree d such that equation 6.4 holds. We can collect all these q_k s in a vector \mathbf{q} of the form

$$\mathbf{q} = \begin{pmatrix} q_1(x) \\ q_2(x) \\ \vdots \\ q_m(x) \end{pmatrix} = V \begin{pmatrix} 1 \\ x \\ \vdots \\ x^d \end{pmatrix} = V\mathbf{x}, \quad V \in \mathbb{R}^{m \times (d+1)} \quad (6.7)$$

and thereby rewrite equation 6.4 as

$$p(x) = \sum_{k=1}^m q_k(x)^2 = (V\mathbf{x})^T V\mathbf{x} = \mathbf{x}^T V^T V\mathbf{x} \equiv \mathbf{x}^T Q\mathbf{x} \quad (6.8)$$

where $Q \equiv V^T V$. From this, one immediately obtains the following

Lemma 1. *Let $p(x)$ be a univariate polynomial of degree $2d$. Then $p(x)$ is a sum of squares if and only if there exists a real, symmetric matrix $Q \in S^{d+1}$ that satisfies*

$$p(x) = \mathbf{x}^T Q\mathbf{x} \text{ and } Q \succeq 0 \quad (6.9)$$

Proof. The forward direction follows by construction. As $p(x)$ is a sum of squares, it has to be non-negative and therefore

$$\forall \mathbf{x} : \mathbf{x}^T Q\mathbf{x} \geq 0 \quad (6.10)$$

which, by definition, means that Q is positive-semidefinite: $Q \succeq 0$.

For the backward direction we assume that there exists a real, symmetric and positive-semidefinite matrix Q satisfying $p(x) = \mathbf{x}^T Q\mathbf{x}$. As there is a Cholesky decomposition $A = L^T L$ for every real, symmetric and positive-semidefinite matrix A , we can factor $Q = V^T V$ and thereby obtain a sos-decomposition for $p(x)$. \square

Figuring out if such a matrix exists is an instance of an SDP problem: Check if there is a matrix Q satisfying the constraints $Q \succeq 0$ and $p_k = \sum_{i+j=k} Q_{ij}$ for $k = 1, \dots, 2d$.

6.2.2. Multivariate Polynomials

For the multivariate case, we consider a polynomial of degree $2d$ in n variables:

$$p(x_1, \dots, x_n) = \sum_{\substack{\alpha_1, \dots, \alpha_n \\ \alpha_1 + \dots + \alpha_n \leq 2d}} p_{\alpha_1, \dots, \alpha_n} (x_1^{\alpha_1} \cdots x_n^{\alpha_n}) \quad (6.11)$$

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As we can choose any combination of up to $2d$ elements from a set of $n + 1$ elements $1, x_1, \dots, x_n$ the polynomial consists of $\binom{n+2d}{2d}$ terms. By defining

$$\mathbf{x} = (1, x_1, \dots, x_n, x_1^2, x_1x_2, \dots, x_n^d) \quad (6.12)$$

as the vector of all the $\binom{n+d}{d}$ monomials of degree d or smaller, we can proceed analogously to the previous section and obtain the following

Theorem 2. *A multivariate polynomial $p(x_1, \dots, x_n)$ in n variables and of degree $2d$ is a sum of squares if and only if there exists a real, symmetric matrix $Q \in S^{\binom{n+d}{d}}$ satisfying*

$$p_\alpha = \sum_{\beta+\gamma=\alpha} Q_{\beta\gamma} \text{ and } Q \succeq 0 \quad (6.13)$$

where $\alpha = (\alpha_1, \dots, \alpha_n)$, $\beta = (\beta_1, \dots, \beta_n)$ and $\gamma = (\gamma_1, \dots, \gamma_n)$.

This corresponds to a semidefinite programming problem with $\binom{n+2d}{2d} + 1$ constraints.

6.3. Application to Bell Inequalities

To apply the results from the previous sections to our problem, we first have to rewrite the Bell operator in terms of matrices: $B = \langle C, X \rangle$ with the so-called *moment matrix* $X = \mathbf{xx}^\dagger$ where \mathbf{x} is a vector of the operators $A_{j_1}^{(i_1)} \cdots A_{j_k}^{(i_k)}$. As the operators do not commute in general, the Bell operator is a non-commutative polynomial. Some of the operators also obey certain relations, such as $A_j^{(i)} A_j^{(i)} = 1$, which can be written in terms of matrix equalities $\langle \tilde{A}_i, X \rangle = b_i$.⁴ This way we obtain the SDP problem

$$\begin{aligned} & \text{minimise: } \langle C, X \rangle \\ & \text{subject to: } X \succeq 0 \\ & \langle \tilde{A}_i, X \rangle = b_i \end{aligned}$$

Running the programme produces a maximal dual solution $b = \mathbf{b}^T \mathbf{y}$ and thereby a lower bound on B . Due to the weak duality this solution satisfies

$$B - b = \langle C, X \rangle - \mathbf{b}^T \mathbf{y} = \langle C - \underbrace{\sum_{i=1}^m \tilde{A}_i y_i}_Q, X \rangle \geq 0 \quad (6.14)$$

The programme also gives out the matrix $Q \equiv C - \sum_{i=1}^m \tilde{A}_i y_i \succeq 0$ ⁵, which we can use to rewrite $(B - b)$ as a sum of squares:

⁴ \tilde{A}_i is introduced to rewrite the relations between the operators in \mathbf{x} in terms of matrix equalities and should not be confused with the operators themselves.

⁵ Q is positive-semidefinite, because the dual problem is constrained by $\sum_{i=1}^m \tilde{A}_i y_i \preceq C$.

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$$B - b = \langle Q^T, X \rangle = \text{Tr}(Q(\mathbf{x}\mathbf{x}^\dagger)) = \text{Tr}(\mathbf{x}^t Q \mathbf{x}) = \mathbf{x}^t Q \mathbf{x} \quad (6.15)$$

By generating an eigendecomposition of Q we can write it as

$$Q = V D V^T = V \sqrt{D} (V \sqrt{D})^T \equiv W W^T \quad (6.16)$$

Inserting this into equation 6.15 we obtain

$$B - b = \mathbf{x}^t W W^T \mathbf{x} = (W^T \mathbf{x}^*)^T (W^T \mathbf{x}) = \sum_i |w_i^T \mathbf{x}|^2 \quad (6.17)$$

where $w_i = \sqrt{d_i} v_i$ is the i -th column vector of W . Knowing the eigendecomposition of Q we can write down the sos-decomposition for $(B - b)$ and thereby prove that b is indeed a quantum bound for B .

6.3.1. SOS for the CHSH-inequality

Recall that the CHSH-inequality is

$$\langle A_0 B_0 \rangle + \langle A_0 B_1 \rangle + \langle A_1 B_0 \rangle - \langle A_1 B_1 \rangle \geq -2 \quad (6.18)$$

The corresponding Bell operator is $B = A_0 B_0 + A_0 B_1 + A_1 B_0 - A_1 B_1$, whose expectation value can be rewritten as

$$p(x) = \langle C, X \rangle \quad (6.19)$$

for

$$X = \mathbf{x}\mathbf{x}^\dagger, \quad \mathbf{x} = (1, A_0, A_1, B_0, B_1, A_0 B_0, A_0 B_1, A_1 B_0, A_1 B_1)^T \quad (6.20)$$

and a 9×9 matrix

$$C = \frac{1}{4} \left(\begin{array}{c|cc|cccc} 0 & & & & & & & & & \\ & & & 1 & 1 & & & & & \\ & & & 1 & -1 & & & & & \\ \hline & & 1 & 1 & & & & & & \\ & & 1 & -1 & & & & & & \\ \hline & 1 & & & & & & & & \\ & 1 & & & & & & & & \\ & 1 & & & & & & & & \\ & -1 & & & & & & & & \end{array} \right) \quad (6.21)$$

where empty entries correspond to zeros. The operators A_i and B_i obey the relations

$$A_i^2 = B_i^2 = 1 \qquad A_i B_j = B_j A_i \quad (6.22)$$

6. A Method to Generate PPT Bounds

which can be expressed in terms of matrix inequalities

$$\langle \tilde{A}_i, X \rangle = b_i \quad (6.23)$$

To solve the semidefinite programme we used MatLab and the package ‘‘CVX’’, which provides the tools for convex optimisation. The minimum value obtained this way is $b = -2\sqrt{2}$. It is worth noting that one does not need to impose all the constraints to obtain this value. Changing the constraints does, however, change the matrix $Q^T = C - \sum_{i=1}^m \tilde{A}_i y_i$. So we tried adding and removing the constraints until we obtained a relatively simple eigendecomposition of Q . For the following results only the constraints $A_i^2 = B_i^2 = 1 \forall i$ and $A_0 B_1 = B_1 A_0$ were imposed. The eigenvectors corresponding to non-zero eigenvalues of Q are:

$$v_1 = \frac{1}{2}(0, 0, 0, 0, 0, 1, -1, 1, 1)^T \quad \lambda_1 = \frac{1}{2\sqrt{2}} \quad (6.24)$$

$$v_2 = \frac{1}{2}(0, 1, -1, 0, \sqrt{2}, 0, 0, 0, 0)^T \quad \lambda_2 = \frac{1}{\sqrt{2}} \quad (6.25)$$

$$v_3 = \frac{1}{2}(0, 1, 1, \sqrt{2}, 0, 0, 0, 0, 0)^T \quad \lambda_3 = \frac{1}{\sqrt{2}} \quad (6.26)$$

$$v_4 = -\frac{1}{\sqrt{12}}(2\sqrt{2}, 0, 0, 0, 0, 1, 1, 1, -1)^T \quad \lambda_4 = 1.0607 \quad (6.27)$$

Using $B - b = \sum_i \lambda_i |\mathbf{v}_i^T \mathbf{x}|^2$ we can now calculate the sum of squares for the CHSH-inequality:

$$\begin{aligned} B - 2\sqrt{2} &= \frac{1}{8\sqrt{2}}(A_0(B_0 + B_1) - A_1(B_0 - B_1))^2 \\ &+ \frac{1}{4\sqrt{2}}(A_0 - A_1 + \sqrt{2}B_1)^2 \\ &+ \frac{1}{4\sqrt{2}}(A_0 + A_1 + \sqrt{2}B_0)^2 \\ &+ \frac{1}{8\sqrt{2}}(2\sqrt{2} + A_0(B_0 + B_1) + A_1(B_0 - B_1))^2 \end{aligned} \quad (6.28)$$

One can check that this equation holds by expanding the right hand side. With equation 6.28 we have provided an analytical proof that the lower bound on the CHSH inequality is $-2\sqrt{2}$ for all quantum states and for all measurements.

The sum-of-squares-decomposition given by equation 6.28 is also useful when trying to find a particular quantum state $|\psi\rangle$ and a set of measurements that lead to maximal quantum violation. In order to obtain the quantum bound $\langle \psi | B | \psi \rangle = -2\sqrt{2}$ the expectation values of the terms in the parentheses with respect to $|\psi\rangle$ must all be zero. This provides a number of relations that $|\psi\rangle$ and the measurement operators leading to maximal quantum violation of the CHSH-inequality must satisfy.

6.4. Sum of Squares for PPT states

We can now use the results from the previous sections to develop a new method to generate PPT-bounds for a given Bell inequality. The method is based on the following observation: To show that b is a PPT-bound on B it is sufficient to show that $(B - b)$ is a sum of squares S_1 *plus* the partial transpose of another sum of squares S_2 :

$$B - b = S_1 + S_2^{T_i} \quad (6.29)$$

Proof. Let's assume that there exist two sums of squares S_1 and S_2 such that $B - b = S_1 + S_2^{T_i}$. Then

$$\langle B - b \rangle = \text{Tr}(\rho(B - b)) = \text{Tr}(\rho(S_1 + S_2^{T_i})) = \text{Tr}(\rho S_1) + \text{Tr}(\rho S_2^{T_i}) \quad (6.30)$$

Because any density matrix is positive-semidefinite and because $S_1 \succeq 0$, we know that the first term must be non-negative. To see that the second term is non-negative as well, we use that

$$\text{Tr}(\rho S_2^{T_i}) = \sum_{i,j} \rho_{ij} S_{2_{ij}} = \text{Tr}(\rho^{T_i} S_2), \quad (6.31)$$

which is non-negative for any state with a positive partial transpose. From this it follows that $\langle B \rangle \geq b$, proving that b is a valid PPT-bound for the Bell inequality B . □

This leaves more possibilities for the optimisation than in the case where only S_1 is considered, which is why one might find stronger bounds than the quantum bound for B . In particular, one might find that the PPT-bound equals the classical bound, which would mean that the inequality cannot be violated by PPT-states. This is what one would expect if they believed the Peres conjecture to be true. On the other hand, if the PPT-bound does not equal the classical bound, it might be a good candidate to falsify the Peres conjecture. However, it might be possible to improve the PPT-bound by minimising over a larger set of variables, i.e. higher-order products of operators and their transpositions in \mathbf{x} . To do so, one would have to include not only combinations of up to two measurement operators in \mathbf{x} , as we do in the following examples, but also combinations of these combinations and so on. The maximal degree of the monomials in \mathbf{x} defines the *level* of the moment matrix $X = \mathbf{x}\mathbf{x}^\dagger$.

6.4.1. Application to CHSH

To open up the new possibilities for the optimisation in the SDP-programme used in Section 6.3.1, we create the matrix

$$Z = \begin{pmatrix} X & 0 \\ 0 & X^\Gamma \end{pmatrix} \quad (6.32)$$

where Γ denotes the partial transpose and $X = \mathbf{xx}^\dagger$. To capture identities such as $B_0^T B_1^T = (B_1 B_0)^T$ we have to include all the different combinations of two elements of $\{\mathbb{1}, A_0, \dots, B_1^T\}$ in \mathbf{x} . Therefore the matrix $X = \mathbf{xx}^\dagger$ has 98×98 entries⁶, which satisfy quite a number of constraints. Using a C++ programme to generate the matrix inequalities corresponding to the constraints and optimising the Bell operator we obtained $b = -2$ as a PPT-bound for B . This is the classical bound for the CHSH-inequality, so at least in the CHSH-case the Peres conjecture holds. The sum of squares in this case is quite simple:

$$B + 2 = \frac{1}{8}(B + 2)^2 + \frac{1}{8}[(B^T + 2)^2]^T \quad (6.33)$$

Similarly one can show that

$$2 - B = \frac{1}{8}(2 - B)^2 + \frac{1}{8}[(2 - B^T)^2]^T \quad (6.34)$$

So we have obtained a simple proof that for PPT-states the CHSH-inequality is bounded by $-2 \leq \langle B \rangle \leq 2$.

6.4.2. Application to chained inequalities

With equation 6.33 we can also prove that the Braunstein-Caves chained inequalities [BC90] hold. These are Bell inequalities for the scenario $(2, m, 2)$, which can be obtained by adding CHSH-inequalities with different measurement operators:

$$\sum_{i=1}^{m-1} \langle A_0 B_{i-1} + A_{i-1} B_{i-1} + A_{i-1} B_{i-2} - A_0 B_{i-2} \rangle \geq 2(m-1) \quad (6.35)$$

The CHSH-inequalities in the sum can be obtained from equation 3.18 with the transformations

$$A_0 \rightarrow -A_0, \quad A_1 \rightarrow A_{i-1}, \quad B_0 \rightarrow B_{i-2}, \quad B_1 \rightarrow B_{i-1}. \quad (6.36)$$

As we already know the decomposition of $(B_{CHSH} - 2)$ into a sos plus the partial transpose of another sos, we can prove that the chained inequalities are satisfied for PPT-states by inserting this decomposition into equation 6.35.

⁶We have nine elements $(\mathbb{1}, A_0, A_1, B_0, B_1, A_0^T, A_1^T, B_0^T, B_1^T)$ with $9^2 = 81$ possible combinations. But $\mathbb{1}A_i/B_i = A_i/B_i\mathbb{1}$, $A_i A_i = B_i B_i = \mathbb{1}$ and $A_i B_j = B_j A_i$ so we get $81 - 8 - 8 - 16 = 49$ entries for each of the matrices X and X^T .

7. Results

In this chapter we present the results we obtained by applying the methods developed in the previous sections to a particular Bell scenario. For our studies, we considered a simplified local polytope for the $(3, 2, 2)$ -scenario with outcomes $d \in \{+1, -1\}$. As mentioned before, the local polytope for $(3, 2, 2)$ is constrained by over 50000 Bell inequalities [PS01]. One can, however, reduce the number of inequalities drastically, by considering a projection of this polytope.

7.1. The Projected Polytope

The dimension of the local polytope for $(3, 2, 2)$ is

$$D = [m(d-1) + 1]^n - 1 = 26. \quad (7.1)$$

It is described by vectors of 26 probabilities or equally, as shown in section 4.2.1, by vectors of 26 correlators. By considering only one- and two-body correlators, we projected the local polytope onto a smaller polytope of dimension 18.¹

$$\begin{array}{l} \mathbf{p} = (\langle A_0 \rangle, \dots, \langle B_1 C_1 \rangle, \dots, \langle A_1 B_1 C_1 \rangle)^T \\ \mathbf{p} = (\langle A_0 \rangle, \dots, \langle B_1 C_1 \rangle)^T \end{array}$$

Figure 7.1.: Projection onto the local polytope of only one- and two-body correlators.

Just like the full local polytope, the projected polytope is the convex hull of the points corresponding to local deterministic strategies. These points can be generated by assigning one of the two possible outcomes to each of the one-body correlators and computing the values of the two-body correlators via $\langle A_i B_j \rangle = \langle A_i \rangle \langle B_j \rangle$, $\langle B_i C_j \rangle = \langle B_i \rangle \langle C_j \rangle$ and $\langle A_i C_j \rangle = \langle A_i \rangle \langle C_j \rangle$ for $i, j \in \{0, 1\}$. There are 2^6 such extremal points, which we generated with a C++ programme. This way, we obtained a full vertex-description of the local polytope. Then we used the software *polymake* to generate the corresponding inequalities via Fourier-Motzkin elimination. As a result we obtained 5864 inequalities - few compared to the full polytope for $(3, 2, 2)$ with 53856 [PS01] inequalities, yet still far too many to analyse in detail.

¹One can see straightforwardly that the dimension of the projected polytope is 18 by writing down all of the possible one- and two-body correlators: $\langle A_0 \rangle, \langle A_1 \rangle, \langle B_0 \rangle, \langle B_1 \rangle, \langle C_0 \rangle, \langle C_1 \rangle, \langle A_0 B_0 \rangle, \langle A_0 B_1 \rangle, \langle A_0 C_0 \rangle, \langle A_0 C_1 \rangle, \langle A_1 B_0 \rangle, \langle A_1 B_1 \rangle, \langle A_1 C_0 \rangle, \langle A_1 C_1 \rangle, \langle B_0 C_0 \rangle, \langle B_0 C_1 \rangle, \langle B_1 C_0 \rangle, \langle B_1 C_1 \rangle$.

7.2. Classes of Bell Inequalities

However, many of these inequalities can be converted into each other by renaming parties, renaming the observables of one party and renaming the outcomes of one observable. Using the breadth-first search algorithm, we grouped all of the 5864 inequalities into nine classes. As explained in Section 5, it is sufficient to analyse one of the inequalities in each class to obtain results that are valid for all inequalities belonging to the same class. The inequalities we chose to analyse are listed in Table 7.1.

class	Bell inequality
1	$\langle A_1 - B_0 + B_1 - C_0 - A_1B_0 + A_1B_1 - A_1C_0 + B_0C_0 + B_0C_1 - B_1C_0 + B_1C_1 \rangle \geq -3$
2	$\langle A_0 - A_1 - 2B_0 - C_0 - C_1 - A_0B_0 + A_0B_1 - A_0C_0 + A_1B_0 + A_1B_1 + A_1C_1 + B_0C_0 + B_0C_1 - B_1C_0 + B_1C_1 \rangle \geq -4$
3	$\langle -A_0 - B_0 - C_0 - C_1 + A_0B_0 + A_0B_1 + A_0C_1 - A_1B_0 + A_1B_1 - A_1C_0 + A_1C_1 + B_0C_0 - B_1C_0 + B_1C_1 \rangle \geq -4$
4	$\langle -2A_1 + B_0 - 2B_1 - 2C_0 - C_1 + A_0B_0 + A_0B_1 - A_0C_0 + A_0C_1 - A_1B_0 + 2A_1B_1 + 2A_1C_0 + A_1C_1 - 2B_0C_0 + B_0C_1 + B_1C_0 + 2B_1C_1 \rangle \geq -6$
5	$\langle -A_0 + A_1 + A_0B_1 - A_0C_0 + A_0C_1 + A_1B_1 - A_1C_0 + A_1C_1 - B_0C_0 - B_0C_1 - B_1C_0 + B_1C_1 \rangle \geq -4$
6	$\langle B_0 + B_1 - C_0 + C_1 - A_0B_0 + A_0B_1 - A_1C_0 - A_1C_1 - B_0C_0 + B_0C_1 - B_1C_0 + B_1C_1 \rangle \geq -6$
7	$\langle A_0 + C_1 + A_0C_1 \rangle \geq -1$
8	$\langle A_0C_0 + A_0C_1 - A_1C_0 + A_1C_1 \rangle \geq -2$
9	$\langle A_0B_0 + A_0C_1 + B_0C_1 \rangle \geq -1$

Table 7.1.: Bell Inequalities including only one- and two-body correlators for $(3, 2, 2)$.

7.3. Quantum and PPT-bounds.

We then computed the quantum and PPT-bounds for the inequalities above, using the method introduced in Chapter 6 and moment matrices of level two. The results are given in Table 7.2.

We found that the only inequalities for which the PPT-bound equals the classical bound are those in classes seven, eight and nine. The inequalities belonging to classes seven and nine can be written as sums of squares and are therefore fulfilled for all quantum states.

$$1 + A_0 + C_1 + A_0C_1 = \frac{1}{4}(1 + A_0 + C_1 + A_0C_1)^2 \geq 0 \quad (7.2)$$

$$1 + A_0B_0 + A_0C_1 + B_0C_1 = \frac{1}{4}(1 + A_0B_0 + A_0C_1 + B_0C_1)^2 \geq 0 \quad (7.3)$$

7. Results

class	classical bound	quantum bound	PPT-bound
1	-3	$-3.82843 \cong -1 - 2\sqrt{2}$	-3.5
2	-4	-4.84337	-4.83249
3	-4	$-4.82843 \cong -2 - 2\sqrt{2}$	-4.74392
4	-6	-7.13719	-7.04822
5	-4	$-4.82843 \cong -2 - 2\sqrt{2}$	-4.5
6	-4	-4.5	-4.5
7	-1	-1	-1
8	-2	$-2\sqrt{2}$	-2
9	-1	-1	-1

Table 7.2.: Bounds for the Bell inequalities for $(3, 2, 2)$ and moment matrices of level $n = 2$.

The equations belonging to class eight, on the other hand, are simply different versions of the CHSH inequality, whose decomposition we already know from equation 6.33:

$$\begin{aligned}
 A_0C_0 + A_0C_1 - A_1C_0 + A_1C_1 + 2 &= \frac{1}{8}(A_0C_0 + A_0C_1 - A_1C_0 + A_1C_1 + 2)^2 \\
 &+ \frac{1}{8}[(A_0C_0 + A_0C_1 - A_1C_0 + A_1C_1)^T + 2]^2 \quad (7.4)
 \end{aligned}$$

For all of the other inequalities in classes one to six, the PPT-bound does not equal the classical bound. However, it is possible that this bound can be improved by going to a higher level with respect to the optimisation variable X . This would be numerically more expensive, though.

By improving the algorithms used to generate the results presented in this chapter, one could compute the bounds for higher levels to see if the gap between PPT-bounds and classical bounds decreases. It would also be interesting to apply our method to study scenarios with more parties, measurements or outcomes to get a broader understanding of the connection between PPT-states and local hidden variable models.

8. Conclusion

In this thesis we showed how to separate correlations admitting an LHV-model from nonlocal states via Bell inequalities. By interpreting these Bell inequalities geometrically as the half-spaces constraining a convex polytope, we showed a systematic way to construct all the Bell inequalities for a given scenario. More specifically, we introduced an algorithm, the Fourier-Motzkin elimination, that allowed us to generate Bell inequalities from the set of local deterministic points. These points could be obtained easily by fixing the outcomes for each measurement as a function solely of the input of the corresponding party performing the measurement.

With the BFS-algorithm we were able to group the generated Bell inequalities into classes. As the members of one class can be obtained from a single inequality by successively applying certain symmetry transformations, they do not differ in a physically relevant way. This means that the results obtained for one Bell inequality are valid for all Bell inequalities in its orbit. This drastically reduced the amount of inequalities we had to analyse.

Finally, we expressed the problem of finding the PPT-bound of a given Bell inequality in terms of an SDP-problem. Additionally, we introduced a method allowing us to prove analytically that the computed PPT-bound is valid. Applying this method to the CHSH-inequality, we obtained a simple proof that the Peres conjecture holds both for the CHSH-inequality and the Braunstein-Caves chained inequalities.

We then applied the abovementioned methods to investigate the particular Bell scenario $(3, 2, 2)$. In particular, we generated all the Bell inequalities involving only one- and two-body correlators for this scenario, grouped them into classes and computed quantum and PPT-bounds for each class of inequalities. This method revealed an interesting fact: While for some Bell inequalities it is easy to certify that they cannot be violated by PPT-states, it appears to be more intricate to find such certificates for other Bell inequalities. We think that a characterisation of this interesting property of Bell inequalities would yield new insights into why and in which circumstances the Peres conjecture is false.

A. Measurement Statistics for the Partial Trace

We want to prove that one obtains the same statistics when performing a measurement $M = \mathbb{1} \otimes M_B$ on a composite system $\hat{\rho}_{AB}$ and when performing the measurement M_B on the partial trace $\text{Tr}_A(\hat{\rho}_{AB})$. The most general form of $\hat{\rho}_{AB}$ is

$$\hat{\rho}_{AB} = \sum_i p_{ij}^{kl} |a_i\rangle\langle a_j| \otimes |b_k\rangle\langle b_l| \quad (\text{A.1})$$

Performing the measurement $M = \mathbb{1} \otimes M_B$ on $\hat{\rho}_{AB}$ yields

$$\begin{aligned} p(m) &= \text{Tr}(M\hat{\rho}_{AB}) \\ &= \sum_i p_{ij}^{kl} \text{Tr}(\mathbb{1} |a_i\rangle\langle a_j| \otimes M_B |b_k\rangle\langle b_l|) \\ &= \sum_i p_{ij}^{kl} \underbrace{\text{Tr}(|a_i\rangle\langle a_j|)}_{\delta_{ij}} \cdot \text{Tr}(M_B |b_k\rangle\langle b_l|) \\ &= p_{jj}^{kl} \text{Tr}(M_B |b_k\rangle\langle b_l|). \end{aligned} \quad (\text{A.2})$$

Performing the measurement M_B on $\hat{\rho}_B = \text{Tr}_A(\hat{\rho}_{AB})$ on the other hand yields

$$\begin{aligned} \tilde{p}(m) &= \text{Tr}(M_B \hat{\rho}_B) \\ &= \text{Tr} \left[M_B \cdot \left(\sum_i p_{ij}^{kl} \underbrace{\text{Tr}(|a_i\rangle\langle a_j|)}_{\delta_{ij}} |b_k\rangle\langle b_l| \right) \right] \\ &= p_{jj}^{kl} \text{Tr}(M_B |b_k\rangle\langle b_l|) = p(m). \end{aligned} \quad (\text{A.3})$$

B. Dimension of the No-signalling Polytope

Here we show that the dimension of \mathcal{P}_{NS} is $[(d-1)m+1]^n - 1$. Our proof follows closely the presentation in [Pir05, p.3-4].

Consider the marginals $p(a_{i_0}, \dots, a_{i_q} | x_{i_0}, \dots, x_{i_q})$ for all possible subsets $\{i_1, \dots, i_q\}$ of size q and for all $q = 0, \dots, n-1$. Of these marginals only retain the ones such that $x_i \neq 0$ for all $i \in \{i_1, \dots, i_q\}$. The number of the remaining probabilities can be computed with the following combinatorial considerations: For each subset of i_q s there are m^{q+1} possible combinations of x_i s and $(d-1)^{q+1}$ possible combinations of a_i s. Therefore the probabilities define in total

$$D = \sum_{q=0}^{n-1} \binom{n}{q+1} [(d-1)m]^{q+1} = [(d-1)m+1]^n - 1 \quad (\text{B.1})$$

numbers. Using the normalisation and no-signalling constraints, we can reconstruct all probabilities $p(a_0, \dots, a_{n-1} | x_0, \dots, x_{n-1})$ from the the set of these marginals. Therefore the dimension of the no-signalling polytope is given by D .

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Statement of Authentication

I hereby declare that I have written the present thesis independently and without use of other resources than those indicated.

Handwritten signature of V. Kabel in black ink.

Munich, July 3, 2017