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Geometrical aspects of qudits concerning Bell inequalities

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Abstract

The aim of this thesis is to investigate quantum entanglement and quantum non-locality of bipartite finite-dimensional systems (bipartite qudits). Entanglement is one of the most fascinating non-classical features of quantum theory, and besides its impact on our view of the world, it can be exploited for applications such as quantum cryptography and quantum computing. This circumstance has led to a growing interest and profound investigations in this area. Although entanglement and non-locality are ordinarily regarded as one and the same, under close consideration this cannot be taken for granted. The reason for this is that entanglement is defined by the mathematical structure of a quantum state in a composite Hilbert space, whereas nonlocality signifies that the statistical behaviour of a system cannot be described by a local realistic theory. For the latter it is essential that the correlation probabilities of such theories obey so-called Bell inequalities, which are violated for certain quantum states. The main focus of this thesis is on the comparison of both properties with the objective of understanding their relation. In terms of the analysis of entanglement, recent methods for the detection are presented and discussed. Because of the fact that the correlation probabilities in general depend on the measurement settings it is necessary to optimise these in order to reveal nonlocality. This problem is solved for a particular Bell inequality (CGMLP) by means of a self-developed numerical search algorithm. These methods are then applied to density matrices of a subspace spanned by the projectors of maximally entangled two-qudit states. This set of states has not only interesting properties with respect to our investigations, but also serves to visualise and analyse the state space geometrically.

Kurzfassung

Diese Diplomarbeit setzt sich mit Verschränkung und Nichtlokalität in bipartiten endlich-dimensionalen Systemen (bipartite Qudits) auseinander. Die Verschränkung ist eines der faszinierendsten nichtklassischen Phänomene der Quantentheorie, und neben ihrer Bedeutung für unser Weltbild findet sie Anwendung in der Quantenkryptographie und der Quanteninformatik. Diese Tatsache hat zu wachsendem Interesse und ausgiebiger Forschung auf diesem Gebiet geführt. Verschränkung und Nichtlokalität werden für gewöhnlich als ein und dasselbe angesehen. Jedoch ist dies unter genauer Betrachtung nicht als selbstverständlich hinzunehmen, was daran liegt, dass Verschränkung durch die mathematische Struktur eines Zustands in einem zusammengesetzten Hilbertraum definiert ist. Nichtlokalität hingegen besagt, dass das statistische Verhalten eines Systems nicht durch eine lokal-realistische Theorie beschrieben werden kann. Für letzteres ist wesentlich, dass die Korrelationswahrscheinlichkeiten solcher Theorien sogenannte Bell-Ungleichungen erfüllen, welche jedoch durch bestimmte Quantenzustände verletzt werden. Diese Diplomarbeit dient insbesondere dazu, beide Eigenschaften miteinander zu vergleichen. Für die Untersuchung der Verschränkung werden aktuelle Separabilitätskriterien vorgestellt und diskutiert. Aufgrund der Tatsache, dass die Korrelationswahrscheinlichkeiten im Allgemeinen von der Messsituation abhängen, ist es notwendig diese zu optimieren, um Nichtlokalität nachzuweisen. Dieses Problem wird für eine bestimmte Bell-Ungleichung (CGLMP) durch einen selbstentwickelten numerischen Suchalgorithmus gelöst. Die besprochenen Methoden werden dann auf Dichtematrizen eines Unterraums, aufgespannt durch Projektoren von maximal verschränkten Zwei-Qudit-Zuständen, angewandt. Diese Menge von Zuständen hat nicht nur interessante Eigenschaften im Bezug auf unsere Untersuchungen, sondern dient auch dazu, den Zustandsraum zu visualisieren und geometrisch zu analysieren.

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Introduction

Modern physical theories often contradict human intuition and this especially applies to quantum physics. One of the most sensational quantum phenomena was recognised by Einstein, Podolsky and Rosen in 1935. In their seminal work [1] they presented a physical situation in which quantum theory seems to violate the principles of relativity. Besides the fact that in such a situation best possible knowledge of the whole does not include best possible knowledge of its parts, particles seem to somehow influence each other at the point of measurement, even if these are space-like separated. The theory here predicts a new type of correlations which cannot be understood on the basis of a local realistic description. These correlations have become known as EPR correlations[1]. At that time, their conclusion was that quantum theory must be incomplete. It was thought that this peculiarity can be eliminated through a more fundamental theory based on local hidden variables. Such a formulation has never been found. Furthermore, the existence of such a theory can be revised experimentally via so-called Bell inequality tests. Experimental evidence of EPR correlations in 1982 by Aspect et al. (see [2]) has led to a growing interest in this subject and a new research field named quantum information has emerged. Many useful applications such as quantum teleportation, quantum cryptography and algorithms for quantum computers have been proposed. Entanglement and nonlocality are now being accepted and investigated by various physicists.

Irrespective of intensive research within the last decades, there still remain many open problems from a theoretical point of view and one of the aims of this thesis is to outline several fundamental ones. In this thesis we investigate bipartite qudit systems, i.e. two d-dimensional systems, in order to gain deeper insight into the subject. The motivation for studying such systems arises from the fact that those are the most simple extensions of the two-qubit system to higher dimensions (Another simple extension can be realised via multipartite systems, where the number of qubits is increased). At this point we might anticipate that investigations become more and more unfeasible with increasing dimensions. Systems with continuous dimensions and/or a great number of parties are almost impossible to analyse with current mathematical tools.

The thesis is organised as follows: In Chapter 1, we first provide an introduction to the mathematical framework necessary to study entanglement, followed by a closer examination of how it can be detected, quantified and classified. In Chapter 2, the focus is on the existence of local realistic theories. We discuss Bell inequalities in details, particularly, the CGLMP inequality. As it will be seen, in order to reveal the nonlocality of a quantum state the measurement setup, which can be expressed in the form of a Bell operator $\mathcal{B}$, has to be optimised. In general, this is a very demanding subject and we contribute to the solution of this problem by presenting a self-developed numerical search algorithm. We end this chapter with further remarks on the comparison of entanglement and nonlocality. The purpose of Chapter 3 is to expose the properties of quantum states in a geometric context by applying entanglement detection criteria and our algorithm. The analysis of the state space of bipartite qubits first leads to a tetrahedron and motivated by its attributes we construct its extension for higher dimensions: the magic simplex.

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[1]or simply quantum correlations

1 Entanglement

1.1 Basics

1.1.1 Definition

In this section we introduce the mathematical definition of entanglement using the most common notation of quantum physics - the **Dirac notation**, which utilises bra and ket vectors. As we do not go beyond bipartite systems, we restrict all mathematical definitions to these in order to simplify our considerations. Consequently, all state vectors are elements of a composite Hilbert space $\mathcal{H}^{AB} = \mathcal{H}^A \otimes \mathcal{H}^B$, where $\mathcal{H}^A$ and $\mathcal{H}^B$ are the Hilbert spaces of the two subsystems A and B. All operators acting on $\mathcal{H}^{AB}$ will be elements of the corresponding Hilbert-Schmidt space $\mathcal{H}_{HS}^{AB}$, that is the set of bounded linear operators. We will utilise the Hilbert-Schmidt inner product defined by $\langle A|B \rangle_{HS} = Tr(A^\dagger B)$, which induces the Hilbert-Schmidt norm $\|A\|_{HS} = \sqrt{Tr(A^\dagger A)}$. Usually the operations on the subsystems $\mathcal{H}^A$ and $\mathcal{H}^B$ are attributed to the fictive persons Alice and Bob, respectively. In 1935, Schrödinger recognised that EPR correlations are related to states $\left|\Psi^{AB}\right\rangle \in \mathcal{H}^{AB}$ that cannot be written as tensor products of state vectors $\left|\Psi^A\right\rangle \in \mathcal{H}^A$ and $\left|\Psi^B\right\rangle \in \mathcal{H}^B$. Consider an arbitrary state $\left|\Psi^{AB}\right\rangle \in \mathcal{H}^{AB}$. By choosing a basis $\left\{\left|i^A\right\rangle\right\}$ of $\mathcal{H}^A$ and $\left\{\left|j^B\right\rangle\right\}$ of $\mathcal{H}^B$ any state of $\mathcal{H}^{AB}$ can be written in the form

$$\left|\Psi^{AB}\right\rangle = \sum_{i,j} c_{ij} \left|i^A\right\rangle \otimes \left|j^B\right\rangle \ , \tag{1.1}$$

with $c_{ij} \in \mathbb{C}$ and normalisation $\sum_{i,j} c_{ij}^* c_{ij} = 1$. We call states that can be written in the form

$$\left|\Psi^{AB}\right\rangle = \left|\Psi^A\right\rangle \otimes \left|\Psi^B\right\rangle \tag{1.2}$$

separable. There is a class of states that cannot be written that way and we denote them as non-separable or entangled. A separable state can contain only classical correlations while an entangled state can contain quantum/EPR correlations. The definition implies that a state (of a subsystem) in general cannot be described by a state vector. It follows that open quantum systems need to be described by density matrices. Those also enable us to take into account decoherence and imperfect state preparations in experiments. For the density matrix formalism however, a generalised definition of separability for mixed states is required. If we suppose that a product state, regardless of whether it is pure or mixed remains separable under local operations and classical communication (see §1.4.2) we can infer that a state is separable iff it can be written in the form

$$\rho^{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B \ , \tag{1.3}$$

with $p_i \geq 0$ and $\sum_i p_i = 1$.

1.1.2 The two-qubit system

We start with the two-qubit system which has the minimal number of degrees of freedom essential for entanglement. The qubit stands for a system with a two dimensional Hilbert space $\mathcal{H} = \mathbb{C}^2$ with an orthonormal basis denoted by $\{|0\rangle, |1\rangle\}$

and is therefore the quantum mechanical counterpart of a classical bit. Nevertheless, it should emphasized that there are major differences between the classical bit and the quantum bit. While a classical bit can either have the value 0 or 1 a qubit can in principle store an infinite amount of information because of the infinitely many superpositions of $|0\rangle$ and $|1\rangle$. However, this information is unusable since we cannot distinguish between two non-orthogonal states with a single measurement. Hence, we can only work with superpositions during information processing (quantum computations), the outcome however should be in an eigenstate of the measured observable. It should be mentioned that qubit systems are more than just simple examples of low dimensional quantum systems. This is because of their relevance in quantum optics (polarisation of photons in horizontal $|H\rangle$ or vertical $|V\rangle$ direction) and experiments with spin $\frac{1}{2}$ particles (spin up $|\uparrow\rangle$ or spin down $|\downarrow\rangle$). As we have a two dimensional Hilbert space we need an operator basis with four elements to declare an operator. In many cases it is useful to work with the Pauli operator basis $\{\mathbb{1}, \sigma_1, \sigma_2, \sigma_3\}^2$, that is an orthogonal basis according to the Hilbert-Schmidt inner product $\langle\sigma_k|\sigma_l\rangle_{HS} = 2\delta_{kl}$, $\langle\mathbb{1}|\sigma_l\rangle_{HS} = 0$, $\langle\mathbb{1}|\mathbb{1}\rangle_{HS} = 2$. Any operator can be written in the form

$$O = a_0 \mathbb{1} + \sum_{i=1}^{3} a_i \sigma_i \, , \tag{1.4}$$

with all $a_i \in \mathbb{C}$. In the case of a density matrix $O = \rho$ we write

$$\rho = \frac{1}{2}\left(b_0 \mathbb{1} + \vec{b} \cdot \vec{\sigma}\right) \, , \tag{1.5}$$

which is equivalent to (1.4) and has advantages with respect to the following restrictions

$$b_0 = 1 \, , \tag{1.6}$$

$$\vec{b} \in \mathbb{R}^3 \, , \tag{1.7}$$

$$\|\vec{b}\| \leq 1 \, . \tag{1.8}$$

The first restriction follows from the condition $tr(\rho) = 1$. The second is a necessary condition for ρ to be hermitian. Since ρ also has to be positive semi-definite we get the third restriction by computing $det(\rho) = \frac{1}{4}(1 - \|\vec{b}\|^2)$. ($det(\rho) \geq 0$ is a necessary condition for non-negativity, in our case it is also sufficient because of $tr(\rho) = 1$ it is not possible for ρ to have two negative eigenvalues). As shown from this, the quantum state of a single qubit can be fully described by a three dimensional real vector $\vec{b}$ that lies within a three dimensional sphere with radius 1. Vector $\vec{b}$ is called the Bloch vector and the sphere, Bloch sphere. If the vector lies on the sphere, the state is pure; if it lies inside, the state is mixed. This follows immediately from $det(\rho) = 0$ for $\|\vec{b}\| = 1$, meaning one eigenvalue has to be 0. This implies that the other eigenvalue has to be 1, and consequently the state is pure.

In the following, we discuss systems of two qubits. To describe such systems we need a four-dimensional Hilbert space $\mathcal{H}^{AB} = \mathbb{C}^2 \otimes \mathbb{C}^2$ and we can choose, for example, an orthonormal basis of type $\{|0^A\rangle \otimes |0^B\rangle, |0^A\rangle \otimes |1^B\rangle, |1^A\rangle \otimes |0^B\rangle, |1^A\rangle \otimes |1^B\rangle\}$. If there is no likelihood of confusion we can get rid of the indices A and B and the

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$^2\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0\rangle\langle1| + |1\rangle\langle0|, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i|0\rangle\langle1| + i|1\rangle\langle0|, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\langle0| - |1\rangle\langle1|$

tensor products $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Before we discuss the Pauli operator basis for bipartite qubit systems in detail, we introduce the most well-known entangled states, namely the Bell states

$$\left|\Psi^{\pm}\right\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle \pm |10\rangle\right) , \tag{1.9}$$

$$\left|\Phi^{\pm}\right\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle \pm |11\rangle\right) . \tag{1.10}$$

The reader may convince himself that these states are indeed entangled, to be more precise, these states are maximally entangled as will be seen in our subsequent discussion of entanglement measures in §1.3. One (perhaps unexpected) feature is that they are all equivalent in terms of local unitaries. The application of a unilateral Pauli matrix $\{\sigma_1 \otimes 1, \sigma_2 \otimes 1, \sigma_3 \otimes 1\}$ onto a certain Bell state yields another Bell state (up to a non-relevant global phase)

$$\sigma_1 \otimes 1 \; : \; \left|\Psi^{\pm}\right\rangle \leftrightarrow \left|\Phi^{\pm}\right\rangle , \tag{1.11}$$

$$\sigma_2 \otimes 1 \; : \; \left|\Psi^{\pm}\right\rangle \leftrightarrow \left|\Psi^{\mp}\right\rangle , \tag{1.12}$$

$$\sigma_2 \otimes 1 \; : \; \left|\Phi^{\pm}\right\rangle \leftrightarrow \left|\Phi^{\mp}\right\rangle , \tag{1.13}$$

$$\sigma_3 \otimes 1 \; : \; \left|\Psi^{\pm}\right\rangle \leftrightarrow \left|\Phi^{\mp}\right\rangle . \tag{1.14}$$

In the next section we systemize the above mentioned attribute to get the generalised Bell states in higher dimensional systems. It is certain that properties and applications of Bell states could be further discussed. However, we continue with the analysis of our bipartite qubit system by examining the operators acting on the Hilbert space. As indicated before we now introduce the Pauli operator basis for the four dimensional Hilbert space. Any operator can be written in the form

$$O = \alpha 1 \otimes 1 + \sum_{i=1}^{3} a_i \sigma_i \otimes 1 + \sum_{i=1}^{3} b_i 1 \otimes \sigma_i + \sum_{i,j=1}^{3} c_{ij} \sigma_i \otimes \sigma_j , \tag{1.15}$$

with $\alpha, a_i, b_i, c_{ij} \in \mathbb{C}$. Due to the fact that Pauli matrices are hermitian, it is apparent that $\alpha, a_i, b_i, c_{ij} \in \mathbb{R}$ for all hermitian operators (for example observables or density matrices). Once again we change the notation slightly

$$\rho = c \left(1 \otimes 1 + \vec{r} \cdot \vec{\sigma} \otimes 1 + 1 \otimes \vec{s} \cdot \vec{\sigma} + \sum_{n,m=1}^{3} t_{nm} \sigma_n \otimes \sigma_m\right) , \tag{1.16}$$

and specify the constraints for density matrices

$$c = \frac{1}{4} , \tag{1.17}$$

$$r_i, s_i, t_{nm} \in \mathbb{R} , \tag{1.18}$$

$$\|\vec{r}\|^2 + \|\vec{s}\|^2 + \sum_{n,m=1}^{3} t_{nm}^2 \leq 3 , \tag{1.19}$$

$$Tr\left(|\Psi\rangle\langle\Psi|\rho\right) \geq 0 \qquad \forall |\Psi\rangle \in \mathcal{H}^{AB} . \tag{1.20}$$

The first restriction has to be fulfilled because $Tr(\rho)$ has to be 1. Hermicity of ρ requires restriction two. The condition $Tr(\rho^2) \leq 1$ implies the third one, while the

fourth condition is the non-negativity condition. As a conclusion, we can say that for two qubits any density matrix $\rho \in \mathcal{H}_{HS}^{AB}$ can be fully specified by two real vectors $\vec{r}$ and $\vec{s}$ and a real 3x3 matrix with elements t_{nm}. The vectors $\vec{r}$ and $\vec{s}$ determine the local characteristics of ρ related to the systems A and B, which can be seen by computing the reduced density matrices

$$\rho_A = Tr_B \rho = \frac{1}{2}\left(\mathbb{1} + \vec{r} \cdot \vec{\sigma}\right) \ , \tag{1.21}$$

$$\rho_B = Tr_A \rho = \frac{1}{2}\left(\mathbb{1} + \vec{s} \cdot \vec{\sigma}\right) \ . \tag{1.22}$$

It can be seen that there is no dependence on the parameters t_{nm}, which can be regarded as correlation parameters since they reflect correlations of classical or EPR type. For this reason, the matrix with components t_{nm} is sometimes referred to as a correlation matrix. For a given density matrix ρ all parameters can be obtained by the use of the associated algebra

$$r_i = Tr\left(\sigma_i \otimes \mathbb{1} \cdot \rho\right) \ , \tag{1.23}$$

$$s_i = Tr\left(\mathbb{1} \otimes \sigma_i \cdot \rho\right) \ , \tag{1.24}$$

$$t_{nm} = Tr\left(\sigma_n \otimes \sigma_m \cdot \rho\right) \ . \tag{1.25}$$

1.1.3 Bipartite qudit systems

The investigation of quantum systems with few dimensions with the aim of gaining insight into the fundamental properties of quantum theory has been one of the most seminal concepts of quantum information and has led to interesting observations and countless applications of entanglement. The two-qubit system has allowed us to study entanglement in the absence of mathematical complexity caused by high dimensionality. However, within recent years, the focus has been on entanglement in quantum systems with more degrees of freedom. We now go beyond the familiar two-qubit system and concentrate on the entanglement of bipartite systems with arbitrary dimensions.

The four Bell states have been useful for many quantum algorithms and seminal experiments. There is a very insightful way to generalise those maximally entangled Bell states onto Hilbert spaces $\mathcal{H}^{AB} = \mathbb{C}^d \otimes \mathbb{C}^d$ with any desired $d \geq 2$. The analogue of the $|\Phi^+\rangle$ state in $\mathbb{C}^d \otimes \mathbb{C}^d$ is a state of the form

$$|\Omega_{0,0}\rangle = \frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} |s^A\rangle \otimes |s^B\rangle \ , \tag{1.26}$$

with an arbitrary orthonormal basis $\{|s^A\rangle\}$ of $\mathcal{H}^A$ and $\{|s^B\rangle\}$ of $\mathcal{H}^B$. We briefly recall that Bell states are equivalent in terms of local unitaries. Consider the application of any local unitary transformation $U_A \otimes U_B$ onto $|\Omega_{0,0}\rangle$

$$U_A \otimes U_B |\Omega_{0,0}\rangle = \frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} U_A |s^A\rangle \otimes U_B |s^B\rangle \ . \tag{1.27}$$

Since the transformations $|s'^A\rangle = U_A |s^A\rangle$ and $|s'^B\rangle = U_B |s^B\rangle$ are basis transformations giving the orthonormal basis $\{|s'^A\rangle\}$ of $\mathcal{H}^A$ and $\{|s'^B\rangle\}$ of $\mathcal{H}^B$, the resulting

state is once again a Bell state

$$\frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} \left| s^{\prime A} \right\rangle \otimes \left| s^{\prime B} \right\rangle \ . \tag{1.28}$$

If there are $d^2 - 1$ particular local unitaries that produce additional $d^2 - 1$ mutually orthonormal Bell states starting from $|\Omega_{0,0}\rangle$, we end up with an orthonormal basis of d^2 Bell states. Local unitaries with such properties are the **Weyl operators**, defined by the action

$$W_{k,l} \left| s \right\rangle = w^{k(s-l)} \left| (s-l) \text{mod } d \right\rangle \ , \tag{1.29}$$

$$w = e^{i 2\pi/d} \ , \tag{1.30}$$

with $k, l \in \{0, ..., d-1\}$. The complete transformation on $\mathcal{H}^{AB}$ is given by $W_{k,l} \otimes \mathbb{1}$, producing d^2 orthonormal **generalised Bell states**

$$|\Omega_{k,l}\rangle = (W_{k,l} \otimes \mathbb{1}) |\Omega_{0,0}\rangle \ . \tag{1.31}$$

We give the explicit verification of orthonormality

$$\langle \Omega_{m,n} | \Omega_{k,l} \rangle = \frac{1}{d} \sum_{r,s=0}^{d-1} \langle (r-n) \text{mod } d | \otimes \langle r | \, w^{-m(r-n)} w^{k(s-l)} | (s-l) \text{mod } d \rangle \otimes | s \rangle$$

$$= \frac{1}{d} \sum_{r,s=0}^{d-1} w^{k(s-l)-m(r-n)} \langle (r-n) \text{mod } d | (s-l) \text{mod } d \rangle \underbrace{\langle r | s \rangle}_{=\delta_{rs}}$$

$$= \frac{1}{d} \sum_{s=0}^{d-1} w^{k(s-l)-m(s-n)} \underbrace{\langle (s-n) \text{mod } d | (s-l) \text{mod } d \rangle}_{\delta_{nl}}$$

$$= \delta_{nl} \frac{1}{d} \sum_{s=0}^{d-1} w^{k(s-l)-m(s-l)}$$

$$= \delta_{nl} \frac{1}{d} \sum_{s=0}^{d-1} w^{(k-m)(s-l)}$$

$$= \delta_{nl} \delta_{km} \ . \tag{1.32}$$

Weyl operators obey the Weyl relations

$$W_{j,l} W_{k,m} = w^{kl} W_{j+k,l+m} \ , \tag{1.33}$$

$$W_{k,l}^{\dagger} = W_{k,l}^{-1} = w^{kl} W_{-k,-l} \ . \tag{1.34}$$

Initially, the Weyl operators were rather contrived for the quantization of classical kinematics instead of the construction of a basis of orthonormal Bell states for Hilbert spaces $\mathcal{H}^{AB} = \mathbb{C}^d \otimes \mathbb{C}^d$. In §3.2 we discuss how this has to be understood and how this concept can help us understand the symmetries and equivalences of quantum states. Since we are now able to construct a basis of Bell states, we continue with seeking a practical operator basis for $\mathcal{H}_{HS}^{AB}$. For qubits, the Pauli operator basis has led to a simple presentation of density matrices via Bloch vectors. For qudits, we once again expand operators in the form

$$O = a_0 \mathbb{1} + \sum_{i=1}^{d^2-1} a_i \Gamma_i \ , \tag{1.35}$$

with the $d \times d$ matrices $\{\mathbb{1}, \Gamma_1, ..., \Gamma_{d^2-1}\}$ forming an orthogonal operator basis $\mathcal{H}_{HS}^{AB}$. If we impose the operators $\{\Gamma_i\}$ to be traceless we can fix the parameter $a_0 = \frac{1}{d}$ for density matrices because of the constraint $Tr\rho = 1$, just as we did for qubits

$$\rho = \frac{1}{d}\mathbb{1} + \sum_{i=1}^{d^2-1} a_i \Gamma_i \ . \tag{1.36}$$

It remains open to show which $\{\Gamma_i\}$ are beneficial for computations and parameterisations. There are various candidates and we want to discuss two of them, namely the **generalised Gell-Mann matrix basis** and the **Weyl operator basis**. Both coincide with the Pauli operator basis for dimension two. We start with the definition of the generalised Gell-Mann (GGM) matrices. For every dimension d we have $d^2 - 1$ matrices divided into three groups:

1. $\frac{d(d-1)}{2}$ symmetric GGM matrices

$$\Lambda_s^{jk} = |j\rangle \langle k| + |k\rangle \langle j| \qquad\qquad 0 \le j < k \le d-1 \tag{1.37}$$

2. $\frac{d(d-1)}{2}$ antisymmetric GGM matrices

$$\Lambda_a^{jk} = -i |j\rangle \langle k| + i |k\rangle \langle j| \qquad\qquad 0 \le j < k \le d-1 \tag{1.38}$$

3. $(d-1)$ diagonal GGM matrices

$$\Lambda^l = \sqrt{\frac{2}{(l+1)(l+2)}} \left(\sum_{j=0}^{l} |j\rangle \langle j| - (l+1) |l+1\rangle \langle l+1| \right) \qquad 0 \le l \le d-2 \tag{1.39}$$

The definitions imply that they are all hermitian and traceless. For proof of orthogonality please refer to [6]. Due to hermicity of the GGM matrices all expansion coefficients have to be reals $a_i \in \mathbb{R}$ for hermitian operators, furthermore for density matrices we can again assign a real $d^2 - 1$ dimensional Bloch vector

$$\rho = \frac{1}{d}\mathbb{1} + \vec{b_\Lambda} \cdot \vec{\Lambda} \ , \tag{1.40}$$

with Bloch vector $\vec{b_\Lambda} = \left(\{b_s^{jk}\}, \{b_a^{jk}\}, \{b^l\} \right)$ and $\vec{\Lambda} = \left(\{\Lambda_s^{jk}\}, \{\Lambda_a^{jk}\}, \{\Lambda^l\} \right)$, with restrictions for j, k, l given in the definitions of the GGM matrices. The vector lies within the **Bloch hypersphere** which precisely means $\|\vec{b_\Lambda}\| \le \sqrt{(d-1)/2d}$, originating from the constraint $Tr(\rho^2) \le 1$ for density matrices. While for dimension two, all vectors within the sphere result in positive semi-definite operators ρ, whereas in higher dimensions this is not the case. This means that there are areas within the sphere that are restricted for density matrices because of resulting $\rho < 0$. Unfortunately, until now no general expression or parametrisation has been found to avoid the holes within the sphere. Hence, this criterion has to be checked separately. The alternative, namely the **Weyl operator basis** is given by the matrices introduced in (1.29) leading to

$$W_{kl} = \sum_{s=0}^{d-1} e^{\frac{2\pi i}{d} sk} |s\rangle \langle (s+l) \bmod d| \qquad\qquad k, l \in \{0, ..., d-1\} \ . \tag{1.41}$$

Once again, we have the unity $W_{00} = \mathbb{1}$ and $d^2 - 1$ additional matrices forming a basis of mutually orthogonal operators. The proof of orthogonality is very similar to (1.32) and can be found in [6]. Hence, in the Weyl operator basis the Bloch vector expression of any density matrix is

$$\rho = \frac{1}{d}\mathbb{1} + \vec{b_W} \cdot \vec{W} \ , \tag{1.42}$$

with a $d^2 - 1$ dimensional Bloch vector $\vec{b_W}$ and a vector $\vec{W}$ containing all operators W_{kl} except W_{00}. It is clear that one has to take into account the arrangement of the vector components. The main discrepancy between $\vec{b_W}$ and the foregoing Bloch vectors is that the components of $\vec{b_W}$ can be complex and they have to satisfy $b_{-k\,-l} = e^{\frac{2\pi i}{d}kl}b_{kl}^*$ (to be understood modulo d) for hermicity of ρ. This is implied when comparing the definition (1.41) with hermicity $\rho^\dagger = \rho$. As before, the constraint $Tr(\rho^2) \leq 1$ enforces the vector $\vec{b_W}$ to lie within a Bloch hypersphere $\|\vec{b_W}\| \leq \sqrt{(d-1)/d}$. Equal to the vectors $\vec{b_\Lambda}$, not all vectors $\vec{b_W}$ within this sphere are permitted, since some lead to matrices with negative eigenvalues. An expression in terms of the components b_{kl} has not yet been established.

Finally we want to extend our Bloch-type operator expansion (1.35) to bipartite qudit systems. We can do this by generalising the expression (1.15) to

$$O = \alpha \mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{d^2-1} a_i \Gamma_i \otimes \mathbb{1} + \sum_{i=1}^{d^2-1} b_i \mathbb{1} \otimes \Gamma_i + \sum_{i,j=1}^{d^2-1} c_{ij} \Gamma_i \otimes \Gamma_j \ . \tag{1.43}$$

1.2 Detection of entanglement

In §1.1.1 we have introduced the definition of separability and entanglement for pure and mixed states. Even though the distinction is well defined, in practice it is difficult to either find a separable decomposition or to prove that such a decomposition does not exist. For this reason, it is preferable to find operational criteria. As it will be shown, all known methods are either unfeasible or not sufficient to solve the problem completely.

1.2.1 Reduced density matrices of pure states

For all bipartite pure states, a necessary and sufficient criterion for separability arises through the form of the reduced density matrices. It is always possible to change the indexing of expression (1.1), using one index running from 1 to $d_A \cdot d_B$ (dimension of $\mathcal{H}_A$ times dimension of $\mathcal{H}_B$) instead of two indices running from 1 to d_A and 1 to d_B, respectively,

$$\left|\Psi^{AB}\right\rangle = \sum_{i=1}^{d_A \cdot d_B} a_i \left|i^A\right\rangle \otimes \left|i^B\right\rangle \ , \tag{1.44}$$

with elements $\left|i^A\right\rangle \in \mathcal{H}^A$ and $\left|i^B\right\rangle \in \mathcal{H}^B$ of some orthonormal bases. For a given state $\left|\Psi^{AB}\right\rangle$ one can minimise the number of nonzero coefficients a_i by the use of proper orthonormal vectors $\{\left|\widetilde{i^A}\right\rangle\}$ and $\{\left|\widetilde{i^B}\right\rangle\}$ (see [3]). If we change the order of the numeration starting with nonzero coefficients $a_i \neq 0$ for $i \in \{1,..,r\}$ followed by

$a_i = 0$ for $i \in \{r+1, .., d_A \cdot d_B\}$ we end up with the **Schmidt decomposition**

$$\left| \Psi^{AB} \right\rangle = \sum_{i=1}^{r} \sqrt{\lambda_i} \left| \widetilde{i^A} \right\rangle \otimes \left| \widetilde{i^B} \right\rangle \qquad a_i = \sqrt{\lambda_i} \; . \qquad (1.45)$$

with $r \leq \min \{d_A, d_B\}$ and $\{\lambda_i\}$ known as the **Schmidt coefficients**. By computing the partial traces we realise that $\{\lambda_i\}$ are the eigenvalues of the reduced density matrices

$$\rho_A = Tr_B \left(\left| \Psi^{AB} \right\rangle \left\langle \Psi^{AB} \right| \right) = \sum_{i=1}^{r} \lambda_i \left| \widetilde{i^A} \right\rangle \left\langle \widetilde{i^A} \right| \; , \qquad (1.46)$$

$$\rho_B = Tr_A \left(\left| \Psi^{AB} \right\rangle \left\langle \Psi^{AB} \right| \right) = \sum_{i=1}^{r} \lambda_i \left| \widetilde{i^B} \right\rangle \left\langle \widetilde{i^B} \right| \; . \qquad (1.47)$$

Obviously, the resulting density matrices are diagonal and have rank r. Consequently, r is called the **Schmidt rank**. By comparing (1.2) with (1.45) we infer Schmidt rank $r = 1$ for all separable states and $r > 1$ for all entangled states. Since the only density matrices with rank 1 are pure states (they have only one eigenvalue $\lambda_1 = 1$) we come to the conclusion that all separable states result in pure reduced density matrices, while entangled states give mixed ones. Note that for practical purposes it is not necessary to construct the Schmidt decomposition of $\left| \Psi^{AB} \right\rangle$ before tracing out a system because the rank will always be equal due to basis independence of the trace. Hence, we have found a powerful tool to distinguish pure separable states from pure entangled ones since it is trivial to examine the mixedness of a density matrix. To summarise, a necessary and sufficient condition for separability of pure states is given by

$$\left| \Psi^{AB} \right\rangle \text{ is separable} \quad \Leftrightarrow \quad Tr(\rho_{A/B}^2) = 1 \; . \qquad (1.48)$$

1.2.2 Detection via positive maps

As we know, in general a quantum state can only be fully described by a density matrix. Here, for a given state it is more difficult to determine whether it is separable or entangled. We begin with a rather theoretical consideration of necessary and sufficient conditions which was presented by the Horodeckis in 1996 [7].
Consider an operator $\Omega \in \mathcal{H}_{HS}^1$ and a linear map $\Lambda : \mathcal{H}_{HS}^1 \rightarrow \mathcal{H}_{HS}^2$. We say the map Λ is **positive (P)** if it maps any positive operator in $\mathcal{H}_{HS}^1$ into the set of positive operators in $\mathcal{H}_{HS}^2$, in terms of mathematics if $Tr(\Omega \cdot P_1) \geq 0$ implies $Tr(\Lambda(\Omega) \cdot P_2) \geq 0$ for all projectors $P_1 \in \mathcal{H}_{HS}^1$ and $P_2 \in \mathcal{H}_{HS}^2$. Now, consider the extended linear map $[\Lambda \otimes \mathbb{1}_n] : \mathcal{H}_{HS}^1 \otimes \mathcal{M}_n \rightarrow \mathcal{H}_{HS}^2 \otimes \mathcal{M}_n$. Here $\mathcal{M}_n$ stands for the set of the complex matrices n×n and $\mathbb{1}_n$ is the appertaining identity. The map Λ is said to be **completely positive (CP)** if its extension maps any positive operator $\Sigma \in \mathcal{H}_{HS}^1 \otimes \mathcal{M}_n$ into the set of positive operators $\mathcal{H}_{HS}^2 \otimes \mathcal{M}_n$, i.e. $Tr(\Sigma \cdot P_1) \geq 0$ implies $Tr([\Lambda \otimes \mathbb{1}_n] (\Sigma) \cdot P_2) \geq 0$ for all projectors $P_1 \in \mathcal{H}_{HS}^1 \otimes \mathcal{M}_n$ and $P_2 \in \mathcal{H}_{HS}^2 \otimes \mathcal{M}_n$ and all $n \in \mathbb{N}$. It might be a bit surprising that positive maps are not necessarily completely positive. All possible physical transformations are CP maps because the transformation of a density matrix has to result in another valid density matrix. For the solution of our separability problem we recognise the following. Consider a separable state $\rho^{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B$ and a positive map Λ_A (not certainly CP)

inducing $[\Lambda_A \otimes \mathbb{1}_B]$. The mapping of ρ^{AB} gives

$$[\Lambda_A \otimes \mathbb{1}_B] \left(\sum_i p_i \rho_i^A \otimes \rho_i^B \right) = \sum_i p_i \left(\Lambda_A \left(\rho_i^A \right) \right) \otimes \rho_i^B . \qquad (1.49)$$

According to our assumption Λ_A being a positive map $\Lambda_A \left(\rho_i^A \right)$ only has non-negative eigenvalues and the same obviously holds for ρ_i^B. All in all, we have a sum of positive operators weighted with $p_i \geq 0$ yielding a positive operator. Hence for positive maps Λ_A the inequality $[\Lambda_A \otimes \mathbb{1}_B] \left(\rho^{AB} \right) \geq 0$ is a necessary condition for ρ^{AB} to be separable. Furthermore, it can be shown (see [7]) that for every inseparable state ρ there exists a positive map Λ_ρ so that $[\Lambda_\rho \otimes \mathbb{1}] (\rho) < 0$. The existence of such a map Λ_ρ is an impressive matter from a theoretical point of view, but for a given state ρ there is no recipe for how to construct such a mapping. Nevertheless, there are several approved positive maps for the detection of entanglement. One of them is the **reduction map**

$$\Lambda_{red} (\rho) = \mathbb{1} Tr(\rho) - \rho . \qquad (1.50)$$

The positivity of the map can be proven by

$$\langle \Psi | \mathbb{1} Tr(\rho) - \rho | \Psi \rangle = Tr(\rho) \underbrace{\langle \Psi | \Psi \rangle}_{1} - \langle \Psi | \rho | \Psi \rangle \geq 0 \quad \forall | \Psi \rangle \in \{ | \Psi \rangle \, | \, \langle \Psi | \Psi \rangle = 1 \} .$$

$Tr(\rho)$ is the sum of all eigenvalues (all positive or zero for positive operators) and $\langle \Psi | \rho | \Psi \rangle$ can maximally yield the largest eigenvalue, thus the map is positive.
Therefore the **reduction criterion** [8] signifies that a separable state has to fulfill the inequalities

$$\rho_A \otimes \mathbb{1} - \rho_{AB} \geq 0 \quad \text{and} \quad \mathbb{1} \otimes \rho_B - \rho_{AB} \geq 0 , \qquad (1.51)$$

with the reduced density matrices ρ_A and ρ_B.
Another method based on positive maps is called **positive partial transpose (PPT) criterion** [9]. For this criterion the well known transposition is used to determine entanglement. For a given operator A, the transposition is defined by

$$A = \sum_{i,j} a_{ij} | i \rangle \langle j | , \qquad (1.52)$$

$$\Lambda_T(A) = A^T = \sum_{i,j} a_{ij} | j \rangle \langle i | . \qquad (1.53)$$

It is obvious that this map is positive

$$A \text{ is positive} \Rightarrow \langle \Psi | A | \Psi \rangle = \sum_{i,j} a_{ij} \overbrace{\langle \Psi | i \rangle}^{\Psi_i^*} \overbrace{\langle j | \Psi \rangle}^{\Psi_j} \geq 0 \quad \forall | \Psi \rangle \in \{ | \Psi \rangle : \langle \Psi | \Psi \rangle = 1 \} . \qquad (1.54)$$

Choose the vector $| \Psi' \rangle = | \Psi^* \rangle$ and compute

$$\langle \Psi' | A^T | \Psi' \rangle = \langle \Psi^* | A^T | \Psi^* \rangle = \sum_{i,j} a_{ij} \overbrace{\langle \Psi^* | j \rangle}^{\Psi_j} \overbrace{\langle i | \Psi^* \rangle}^{\Psi_i^*} \geq 0 . \qquad (1.55)$$

due to (1.54) this is always true for all $|\Psi'\rangle$, thus transposition is a positive map. As a result, we have found the positive partial transpose criterion. For a given state ρ_{AB} the inequalities

$$\rho_{AB}^{T_A} = \sum_{ijkl} \langle ij| \rho_{AB} |kl\rangle \cdot |k\rangle \langle i| \otimes |j\rangle \langle l| \geq 0 \qquad (1.56)$$

$$\text{and} \quad \rho_{AB}^{T_B} = \sum_{ijkl} \langle ij| \rho_{AB} |kl\rangle \cdot |i\rangle \langle k| \otimes |l\rangle \langle j| \geq 0 \qquad (1.57)$$

are necessary conditions for separability. The PPT criterion is stronger than the reduction criterion in all cases (see [8]). It should be mentioned that in the case of a two-qubit system $\mathcal{H}^{AB} = \mathbb{C}^2 \otimes \mathbb{C}^2$ or a qubit-qutrit system $\mathcal{H}^{AB} = \mathbb{C}^2 \otimes \mathbb{C}^3$ it is also a sufficient criterion (see [7]). Since PPT is not a sufficient criterion for higher dimensional systems, there exist entangled states with positive partial transpose. As shown in §1.4 this feature leads to a phenomenon called **bound entanglement**.
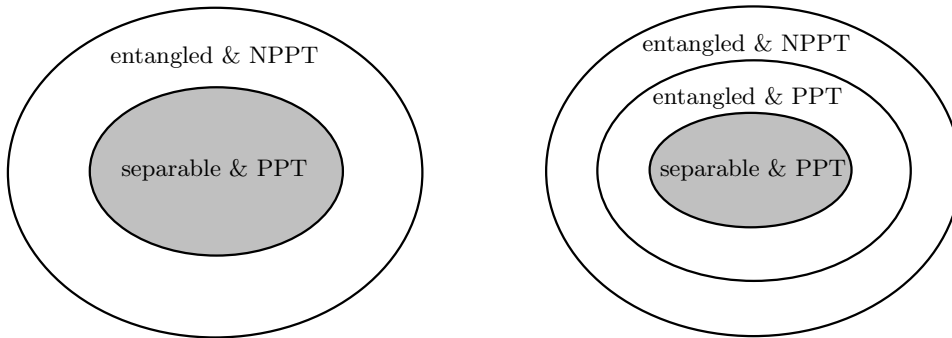

Figure 1.1: Schematic illustration of the set of quantum states of a two-qubit system (left) and higher dimensional systems (right)

1.2.3 Linear contractions criteria

Additional operational criteria can be constructed from contraction mappings [10]. The concept behind those criteria also issues from the extension of maps, but yields criteria that are independent from the previously discussed ones. Consider an operator $\Omega \in \mathcal{H}_{HS}^1$ and a linear map $\Lambda : \mathcal{H}_{HS}^1 \to \mathcal{H}_{HS}^2$. The map Λ is a **contraction** iff it does not increase the Hilbert-Schmidt norm, i.e. $\|\Lambda(\Omega)\|_{HS} \leq \|\Omega\|_{HS}$ holds for all Ω. Once again we define the extension of Λ analogous to the previous section by $[\Lambda \otimes \mathbb{1}_n] : \mathcal{H}_{HS}^1 \otimes \mathcal{M}_n \to \mathcal{H}_{HS}^2 \otimes \mathcal{M}_n$. A map Λ is a **complete contraction** iff it is Hilbert-Schmidt norm non-increasing for all possible extensions $n \in \mathbb{N}$, $\|[\Lambda \otimes \mathbb{1}_n](\Sigma)\|_{HS} \leq \|\Sigma\|_{HS}$ for all $\Sigma \in \mathcal{H}_{HS}^1 \otimes \mathcal{M}_n$. Now, for a separable state

$\rho^{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B$ and a contraction Λ_A we have

$$\begin{aligned}
\left\| [\Lambda_A \otimes \mathbb{1}_B] \left(\rho^{AB} \right) \right\|_{HS} &= \left\| [\Lambda_A \otimes \mathbb{1}_B] \left(\sum_i p_i \rho_i^A \otimes \rho_i^B \right) \right\|_{HS} \\
&\leq \sum_i p_i \underbrace{\left\| \Lambda_A \left(\rho_i^A \right) \right\|_{HS}}_{\leq \left\| \rho_i^A \right\|_{HS} \leq 1} \underbrace{\left\| \rho_i^B \right\|_{HS}}_{\leq 1} \\
&\leq \sum_i p_i = 1 \ . \qquad\qquad\qquad (1.58)
\end{aligned}$$

We have found a necessary condition for separability:

$$\left\| [\Lambda_A \otimes \mathbb{1}_B] \left(\rho^{AB} \right) \right\|_{HS} \leq 1 \ . \qquad\qquad (1.59)$$

Thus, for the detection of entanglement, the relevant maps are the contractions that are not complete contractions. For instance, transposition is such a map. In general there is no common method to construct the whole set of non-complete contractions. One noteworthy criterion based on the idea of contraction surely is the so called **Matrix realignment criterion**, which can detect PPT entanglement in some cases. The basic principle is to use a map $\mathcal{R} : \mathcal{H}_{HS}^{AB} \rightarrow \mathcal{H}_{HS}^2$ that is a contraction for all separable states within the composite Hilbert space $\mathcal{H}_{HS}^{AB}$. While the contraction $[\Lambda_A \otimes \mathbb{1}_B]$ only affects a subspace, the matrix realignment map $\mathcal{R}$ affects the whole space $\mathcal{H}_{HS}^{AB}$ in the following way

$$\mathcal{R}(\rho^{AB}) = \sum_{ijkl} \langle ij | \rho^{AB} | kl \rangle \cdot | i \rangle \langle j | \otimes | k \rangle \langle l | \ . \qquad\qquad (1.60)$$

As we can see realignment interchanges the basis vectors $\{|j\rangle\}$ of $\mathcal{H}^A$ applied on the left-hand side with $\{|k\rangle\}$ of $\mathcal{H}^B$ applied on the right-hand side. This map satisfies

$$\left\| \mathcal{R}(\rho^{AB}) \right\|_{HS} \leq 1 \qquad\qquad (1.61)$$

for all separable states $\rho^{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B$ (see [12]). All states that violate this inequality are necessarily entangled. Some entangled states that slip through the PPT criterion can be detected via the realignment criterion and examples can be found in [11] and [12].

1.2.4 Entanglement witnesses

The last method for the detection of entanglement we discuss are **entanglement witnesses**. They originate from the Hahn-Banach theorem in convex analysis stating that a convex set in a vector space (in our case this is the Hilbert-Schmidt space $\mathcal{H}_{HS}^{AB}$) can be fully described by hyperplanes. In other words, there always exists a hyperplane that separates the convex set from the complement. Based on the fact that a hyperplane can always be expressed by a normal vector W (in our case the vector is an element of $\mathcal{H}_{HS}^{AB}$ and therefore a matrix) and the convexity of the set of separable states, we are able to comprehend a theorem stated by the Horodeckis [7] and B.M. Terhal [13]: A density matrix $\rho_{AB} \in \mathcal{H}_{HS}^{AB}$ is entangled iff there exists a hermitian operator $W \in \mathcal{H}_{HS}^{AB}$ with the properties

$$Tr(W \rho_{AB}) < 0 \ , \qquad\qquad (1.62)$$

$$Tr(W \sigma_{AB}) \geq 0 \ , \qquad\qquad (1.63)$$

for all separable density matrices σ_{AB}. A hermitian operator W accomplishing those requirements is termed an **entanglement witness**. As a consequence, W has to have at least one negative eigenvalue and due to linearity of the trace, nonnegative expectation values on the subset of product states

$$\langle \Psi^A | \otimes \langle \Psi^B | \, W \, | \Psi^A \rangle \otimes | \Psi^B \rangle \geq 0 \qquad \forall \, | \Psi^A \rangle \otimes | \Psi^B \rangle \in \mathcal{H}^{AB} \, . \qquad (1.64)$$

We can rank witnesses W by comparing the sets of entangled states they detect, that is $D_W = \{\rho | Tr(W\rho) < 0\}$. An entanglement witness W_1 is finer than W_2 iff $D_{W_2} \subseteq D_{W_1}$. It is optimal if there is no other entanglement witness which is finer. Hence, an optimal witness $W_{optimal}$ defines a tangent plane to the set of separable states which means that there must be at least one separable σ_{AB} with $Tr(W_{optimal}\sigma_{AB}) = 0$.
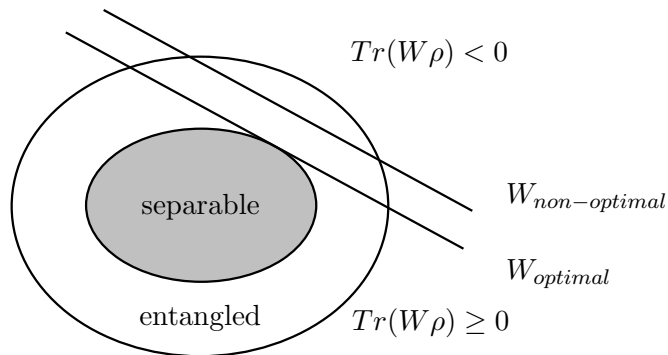

Figure 1.2: Schematic illustration of an optimal and an non-optimal entanglement witness

Further information for the optimisation of entanglement witnesses can be found in [14]. It is evident that a single witness does not detect all entangled states. We only know that for a given entangled state ρ there must be an appertaining entanglement witness W_ρ, an algorithm for the construction however has not yet been established. For this reason entanglement witnesses cannot be seen as a satisfying solution to the separability problem. Furthermore, it is also not clear how many witnesses are necessary to describe the whole set of separable states. Note that if the set is not a polytope then an infinite number of witnesses is required. The geometry of the set depends on the dimension of the considered space or subspace of $\mathcal{H}_{HS}^{AB}$.

1.3 Entanglement measures

The quantification of entanglement is another open problem. This is beyond the separability problem, since the purpose is not only to ascertain if a state is entangled or not, but also to quantify the amount of entanglement within it. This amount should capture the essential features that we associate with entanglement. Before we mention some possible measures we state some requirements on the attributes of a suggestive measure. Take into account that we restrict ourselves to bipartite systems $\mathcal{H}^{AB} = \mathbb{C}^d \otimes \mathbb{C}^d$ with arbitrary dimension d.

1.3.1 The postulates

In the first place, an **entanglement measure** $E(\rho)$ is a mapping of density matrices into the set of positive real numbers

$$\rho \rightarrow E(\rho) \in \mathbb{R}^+ \ . \tag{1.65}$$

Normalisation is not necessary but reasonable and we therefore set

$$E(|\Omega_{k,l}\rangle \langle \Omega_{k,l}|) = log_2(d) \tag{1.66}$$

for the Bell states $|\Omega_{k,l}\rangle$. This should also be the highest value reachable, because we anticipate them to be maximally entangled due to maximal mixedness of their reduced density matrices $\rho_A = \rho_B = \frac{1}{d}\mathbb{1}$, which is unique for pure states

$$0 \leq E(\rho) \leq log_2(d) \ . \tag{1.67}$$

By definition, the outcome of $E(\rho)$ must be zero for all separable states ρ_{sep}

$$E(\rho_{sep}) = 0 \ . \tag{1.68}$$

The most important requirement is **monotonicity under LOCC**. Entanglement cannot be created by local operations and classical communication (§1.4.2), hence the contained amount has to be non-increasing under such transformations

$$E\left(\Lambda_{LOCC}(\rho)\right) \leq E\left(\rho\right) \ . \tag{1.69}$$

This implies that in the special case of local unitaries the outcome of $E(\rho)$ will be invariant [15]

$$E\left(U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger\right) = E\left(\rho\right) \ . \tag{1.70}$$

These postulates are the only ones necessarily required and universally accepted. Some people tend to put further restrictions on entanglement measures. Some of them seem very natural and others can bring mathematical simplicity. One of them is **convexity**

$$E\left(\sum_i p_i\rho_i\right) \leq \sum_i p_i E\left(\rho_i\right) \ . \tag{1.71}$$

Convexity seems to be plausible as we cannot increase entanglement by mixing states and mixtures of entangled states can result in separable states (see §3). **Asymptotic continuity** is another optional restriction

$$\lim_{n\to\infty} \|\rho_n - \sigma_n\|_{HS} \to 0 \Rightarrow \lim_{n\to\infty} |E\left(\rho_n\right) - E\left(\sigma_n\right)| \to 0 \ . \tag{1.72}$$

The interesting thing is that along with the next limitation called **additivity** we can obtain a unique measure for pure states [15]. The additivity is separated in three types. We first consider **partial additivity**

$$E(\rho^{\otimes n}) = nE(\rho) \ , \tag{1.73}$$

which is the weakest addivity criterion. It only reveals that the entanglement content grows linearly with the number of pairs. We may expect that it is reasonable to

assume **full additivity** (following formula with an equal sign). However, it turned out that this would exclude some appreciated measure candidates. The weakened version is the **subadditivity**

$$E(\rho \otimes \sigma) \leq E(\rho) + E(\sigma) \ . \tag{1.74}$$

A more detailed analysis of the postulates and thermodynamical analogies can be found in [16], [17] and [18]. As mentioned before, the additional constraints of partial additivity and asymptotic continuity, inevitably require the measure to coincide with the **von Neumann entropy** S_{vN} of the reduced density matrix $\rho^{A/B} = Tr_{B/A}\left(\rho^{AB}\right)$ for a pure state ρ^{AB}

$$E_{vN}(\rho^{AB}) = S_{vN}\left(\rho^{A/B}\right) = -Tr\left(\rho^A log_2\left(\rho^A\right)\right) = -Tr\left(\rho^B log_2\left(\rho^B\right)\right) \ . \tag{1.75}$$

This is the **uniqueness theorem of entanglement measures** [19].

1.3.2   Measures based on distance

The most intuitive measures are the ones based on distance. The concept is to regard the distance $\mathcal{D}$ of a state $\rho \in \mathcal{H}_{HS}^{AB}$ to the closest separable state $\sigma \in \mathcal{S} \subset \mathcal{H}_{HS}^{AB}$ as the contained amount of entanglement

$$E(\rho) = \inf_{\sigma \in \mathcal{S}} \mathcal{D}\left(\rho, \sigma\right) \ . \tag{1.76}$$

It is apparent that those measures guarantee $E(\rho) = 0$ for separable states. There are several types of possible distance functions $\mathcal{D}$. They do not have to fulfill all criteria for a metric in a mathematical sense, but should meet the requirements of an entanglement measure. Let us consider the **relative entropy of entanglement** which was introduced by Vedral et al. [20]

$$E_R(\rho) = \inf_{\sigma \in \mathcal{S}} Tr\left(\rho\left(log_2\rho - log_2\sigma\right)\right) \ . \tag{1.77}$$

The distance used here does not meet the requirements of a metric because it is not symmetric and does not satisfy the triangle inequality. This is acceptable since relative entropy satisfies all criteria of an entanglement measure including asymptotic continuity and partial additivity (see [21]). Another distance is induced by the Hilbert-Schmidt norm and was investigated in [22]. The resulting measure is called **Hilbert-Schmidt measure** or **Hilbert-Schmidt entanglement**

$$E_{HS}(\rho) = \inf_{\sigma \in \mathcal{S}} \|\rho - \sigma\|_{HS}^2 \ . \tag{1.78}$$

This measure has a different scaling than most of the other candidates because no logarithm is taken. For this reason, it is not common to normalise this function in the foregoing way. Up to now it has not been proven that monotonicity under LOCC is accomplished, meaning it is not clear if it is a good measure of entanglement (see [21],[23]).

1.3.3   Convex roof measures

The idea of convex roof measures is to use entanglement measures for pure states E_{pure} and generalize them to mixed ones in the following way

$$E(\rho) = \inf_{\rho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|} \sum_i p_i E_{pure}\left(|\Psi_i\rangle\langle\Psi_i|\right) \ , \tag{1.79}$$

where the infimum is taken over all possible decompositions of $\rho = \sum_i p_i |\Psi_i\rangle \langle \Psi_i|$ with $\sum_i p_i = 1$ and $p_i \geq 0$. The decomposition yielding the infimum is then said to be the **optimal decomposition** or **optimal ensemble** of ρ. It can be shown that if the utilised measure for pure states E_{pure} is monotonous under LOCC then the induced convex roof measure has this property too (see [5]). The first measure of this kind was **entanglement of formation** E_F with the von Neumann entropy of the reduced density matrices as a measure for pure states $E_{pure} = E_{vN}$ introduced in (1.75)

$$E_F(\rho) = \inf_{\rho = \sum_i p_i |\Psi_i\rangle \langle \Psi_i|} \sum_i p_i E_{vN} \left(|\Psi_i\rangle \langle \Psi_i| \right) \; . \tag{1.80}$$

When this measure was introduced by Bennett et al.[24], the notion was to quantify the amount of pure Bell states that is needed per copy to construct ρ. In other words, N copies of ρ can be prepared out of a minimum of $E_F(\rho) \cdot N$ Bell states and $(1 - E_F(\rho)) \cdot N$ separable states. $E_F(\rho)$ can then be regarded as the contained amount of entanglement. The naming "entanglement of formation" is referable to this concept.

1.4 Bound entanglement

In the previous sections we frequently used the term **local operations and classical communication (LOCC)**. Nevertheless, we neither explained its meaning nor given an adequate mathematical definition. This section will serve as an introduction to this issue. After introducing the class of **quantum operations**, we consider the restrictions for the class of LOCC. Consequences for the purification of entanglement will be briefly discussed, enabling us to justify the term **bound entanglement**.

1.4.1 Quantum operations

We investigate the fundamental quantum operations (see [19], [25]). Our objects of interest are the maps that transform a given state $\rho \in \mathcal{H}_{HS}^1$ into another $\rho' \in \mathcal{H}_{HS}^2$

$$\Lambda : \mathcal{H}_{HS}^1 \rightarrow \mathcal{H}_{HS}^2 \; , \tag{1.81}$$
$$\rho' = \Lambda(\rho) \; . \tag{1.82}$$

As far as we know, any Λ is a combination of four elementary linear maps[3]:

- **Adding an uncorrelated ancilla** $\sigma \in \mathcal{H}_{HS}^2$ to the original quantum system in the state $\rho \in \mathcal{H}_{HS}^1$

$$\Lambda_1 : \mathcal{H}_{HS}^1 \rightarrow \mathcal{H}_{HS}^1 \otimes \mathcal{H}_{HS}^2 \; , \tag{1.83}$$
$$\Lambda_1(\rho) = \rho \otimes \sigma \; . \tag{1.84}$$

- **Tracing out part of the system** in the state $\rho \in \mathcal{H}_{HS}^1 \otimes \mathcal{H}_{HS}^2$

$$\Lambda_2 : \mathcal{H}_{HS}^1 \otimes \mathcal{H}_{HS}^2 \rightarrow \mathcal{H}_{HS}^1 \; , \tag{1.85}$$
$$\Lambda_2(\rho) = Tr_2 \rho \; . \tag{1.86}$$

Here Tr_2 is the partial trace over the Hilbert-Schmidt space $\mathcal{H}_{HS}^2$.

---

[3]It is true that the first two types of transformations are not "real physical" operations, but they are the conversion of experimental operating principles into mathematical diction.

- **Unitary transformations** of a state $\rho \in \mathcal{H}_{HS}^1$

$$\Lambda_3 : \mathcal{H}_{HS}^1 \otimes \to \mathcal{H}_{HS}^1 \ , \tag{1.87}$$

$$\Lambda_3(\rho) = U \rho U^\dagger \ , \tag{1.88}$$

with a unitary operator $U \in \mathcal{H}_{HS}^1$.

- **Measurement of an observable** $A \in \mathcal{H}_{HS}^1$

$$\Lambda_4 : \mathcal{H}_{HS}^1 \to \mathcal{H}_{HS}^1 \ , \tag{1.89}$$

$$\Lambda_4(\rho) = \frac{\sum_i M_i \rho M_i^\dagger}{Tr\left(\sum_i M_i \rho M_i^\dagger\right)} \ . \tag{1.90}$$

Here $\{M_i\}$ is the set of the spectral projectors associated with the eigenvectors of the observable A. It is useful to classify two types of measurements: **Non-selective measurements**, where we work with all outcomes of the measurement and **selective measurements**, where we filter outcomes. Non-selective measurements then yield $\sum_i M_i^\dagger M_i = \mathbb{1}$, and selective measurements $\sum_i M_i^\dagger M_i \leq \mathbb{1}$.

The point of the matter is, that the four maps themselves and their compositions are all completely positive. According to Choi's theorem (see [26]) any map of this type can be expressed in the form

$$\Lambda : \mathcal{H}_{HS}^1 \to \mathcal{H}_{HS}^2 \ , \tag{1.91}$$

$$\Lambda(\rho) = \frac{\sum_i V_i \rho V_i^\dagger}{Tr\left(\sum_i V_i \rho V_i^\dagger\right)} \ , \tag{1.92}$$

with $\rho \in \mathcal{H}_{HS}^1$ (Hilbert-Schmidt space of dimension $n \times n$), $\Lambda(\rho) \in \mathcal{H}_{HS}^2$ (Hilbert-Schmidt space of dimension $m \times m$) and complex matrices $\{V_i\}$ of dimension $m \times n$. This expression is the **Kraus representation** of Λ and the matrices $\{V_i\}$ are the famous **Kraus operators** which obey $\sum_i V_i^\dagger V_i \leq \mathbb{1}$.

1.4.2 Class of LOCC

The concept of **"local operations and classical communication"** stems from quantum communication theory and appears in quantum teleportation, quantum cryptography and distillation protocols. Consider a source and two distant parties A and B, commonly called Alice and Bob. Under realistic circumstances they are able to perform arbitrary quantum operations acting on the particular local Hilbert space $\mathcal{H}^A$ and $\mathcal{H}^B$ and to communicate via classical information. They can neither exchange their quantum systems nor perform "global" transformations involving the entire composite Hilbert space $\mathcal{H}^{AB} = \mathcal{H}^A \otimes \mathcal{H}^B$.
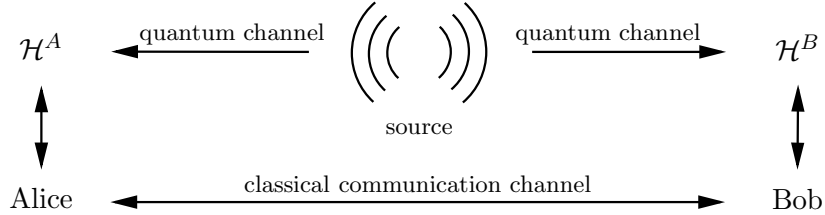

Figure 1.3: Schematic illustration of the LOCC situation

The transcription of this concept into restrictions for the quantum operations §1.4.1 implies that a LOCC operation is a map of the form

$$\Lambda_{AB}(\rho) = \frac{\sum_i (A_i \otimes B_i)\rho(A_i^\dagger \otimes B_i^\dagger)}{Tr\left[\sum_i (A_i \otimes B_i)\rho(A_i^\dagger \otimes B_i^\dagger)\right]} \ , \tag{1.93}$$

with product Kraus operators $\{A_i \otimes B_i\}$ where A_i acts on Alice's Hilbert space $\mathcal{H}^A$ and B_i acts on Bob's Hilbert space $\mathcal{H}^B$. The product Kraus operators reflect that the quantum operations only act locally, while the bilateral dependence of $(A_i \otimes B_i)$ on i reflect that both parties can arrange their actions (they can be classically correlated). While the form of (1.93) is comprehensible, the constraints for the operators $\{A_i \otimes B_i\}$ and their relations can be quite complex. Those depend on the considered communication class, which can be "no communication", "one-way communication" or "two-way communication" (see [5],[19],[25]). The form of (1.93) induces the definition of separable density matrices (1.3).

1.4.3 Distillation and bound entanglement

Outstanding procedures like quantum cryptography or quantum teleportation require pure Bell states. In practice however, we cannot completely neutralise the interaction with the environment that causes decoherence. In the case of the two distant parties Alice and Bob, the linking quantum channel is therefore said to be noisy. We expect that the occurring state ρ^{AB} is no longer a pure Bell state, originally emitted from the source, but a mixture. We characterise the state ρ^{AB} by its **fidelity** F

$$F = Tr\left(|\Omega_{k,l}\rangle \langle \Omega_{k,l}| \rho^{AB}\right) \ , \tag{1.94}$$

which can be regarded as the remaining content of $|\Omega_{k,l}\rangle \langle \Omega_{k,l}|$ in ρ^{AB}. In order to reconstruct an almost pure Bell state with any desired fidelity close to 1 via LOCC operations we have to execute a so-called **distillation protocol**. The first protocols

for qubits were introduced by Bennett et al. [27]. These are the recurrence, hashing and breeding protocols. The hashing and breeding protocols were later generalised for qudits by Vollbrecht et al. [28]. These will not be discussed in detail, but it should be pointed out that they all have one thing in common: They use several copies of ρ^{AB} and local filtering to obtain a smaller number of nearly maximally entangled pure states. For every protocol there is a lower bound for the fidelity F_{LB} in order to work successfully. It is a challenging task to find more universal (ones with a lower F_{LB}) and faster protocols. Irrespective of this intention, there will always be entangled states that cannot be distilled. The conventional term therefore is **bound entanglement** (see [29]). We have already mentioned that in higher dimensional systems there are entangled states which cannot be detected via the PPT criterion. Let us consider how such a state behaves under a LOCC transformation. According to the assumption $\rho \in \mathcal{H}_{HS}^{AB}$ being an entangled density matrix with positive partial transpose we claim

$$\langle \Psi | \, \rho \, | \Psi \rangle \geq 0 \quad \forall \, | \Psi \rangle \in \mathcal{H}^{AB} \ , \tag{1.95}$$

$$\langle \Psi | \, \rho^{T_B} \, | \Psi \rangle \geq 0 \quad \forall \, | \Psi \rangle \in \mathcal{H}^{AB} \ . \tag{1.96}$$

A LOCC transformation of ρ then yields

$$\widetilde{\rho} = \frac{\sum_i (A_i \otimes B_i) \rho (A_i^\dagger \otimes B_i^\dagger)}{Tr \left[\sum_i (A_i \otimes B_i) \rho (A_i^\dagger \otimes B_i^\dagger) \right]} \ . \tag{1.97}$$

We know that transposition changes the sequence of operators according to $(LMN)^T = N^T M^T L^T$ and in our case hermitian conjugation is simply the combination of transposition and complex conjugation $L^\dagger = (L^*)^T$. Partial transposition on $\mathcal{H}_{HS}^B$ then results in

$$\widetilde{\rho}^{\ T_B} = N \sum_i (A_i \otimes B_i^*) \rho^{\ T_B} (A_i^\dagger \otimes (B_i^*)^\dagger) \ , \tag{1.98}$$

wherein N is a positive real number $N = 1/Tr \left[\sum_i (A_i \otimes B_i) \rho (A_i^\dagger \otimes B_i^\dagger) \right] > 0$. Let us investigate positivity

$$\langle \Psi | \, \widetilde{\rho}^{\ T_B} \, | \Psi \rangle = N \sum_i \overbrace{\langle \Psi | \, (A_i \otimes B_i^*)}^{\langle \Phi_i |} \rho^{T_B} \overbrace{(A_i^\dagger \otimes (B_i^*)^\dagger) \, | \Psi \rangle}^{| \Phi_i \rangle}$$

$$= N \sum_i \underbrace{\langle \Phi_i | \, \rho^{T_B} \, | \Phi_i \rangle}_{\geq 0 \ \forall \ | \Phi_i \rangle \in \mathcal{H}^{AB} \, (1.96)}$$

$$\geq 0 \qquad \forall \, | \Psi \rangle \in \mathcal{H}^{AB} \ . \tag{1.99}$$

This proves that $\widetilde{\rho}^{\ T_B}$ is a positive operator. The conclusion is that a LOCC transformation cannot transform a PPT density matrix into a density matrix that is non-positive after partial transposition **(NPPT)**. We have established that a pure maximally entangled state (NPPT) cannot be distilled from a PPT state, even though it contains some entanglement. This justifies the term **bound entanglement**. The existence of NPPT bound entanglement is controversial and a subject of recent research.

2 Bell inequalities

2.1 Local realism versus quantum mechanics

Since the verification of (special) relativity principles most physicists have believed that any fundamental theory is in compliance with local realism.

Realism is the assumption of the existence of definite values for all possible observables. That is, at each point of time these values genuinely exist, whether we measure them or not. "Ideal" measurements with no or marginal disturbance could therefore reproduce these pre-existing values. As a direct consequence, realistic theories are non-contextual.

Locality reflects the key consequence of relativity, that is all interactions between distant objects are limited to the speed of light. Space-like separated objects are therefore independent of one another.

Local realism is the unification of locality and realism.

As obvious as these assumptions may seem, in 1935 Einstein, Podolsky and Rosen showed that quantum mechanics rejects these principles (see [1]). At this period of time, their conclusion was that quantum mechanics must be incomplete, meaning there must be elements of reality that do not appear in the theory. An introduction of such elements however, should restore local realism. Due to their hiddenness they have been called **local hidden variables**, regardless of whether they are hidden in principle or just in experiments at that time. During this period, evidence had not been found yet, demonstrating that all **local hidden variable theories (LHVT)** are incompatible with the predictions of quantum mechanics in particular experiments. In 1964, John Bell derived that the correlation expectation values of local hidden variable theories fulfill inequalities that can be violated by quantum mechanics (see [30]). Moreover, these **Bell inequalities** enable us to experimentally revise the validity of **either** quantum mechanics **or** a local realistic theory. Before going into further details, it is essential to briefly reconsider why and under which circumstances quantum mechanics is said to be non-local. Nonlocality can be ascribed to entanglement and the measurement problem. This can be best understood by considering the Bohm version of the EPR situation (see [31]). Here, two spin-$\frac{1}{2}$ particles, for example electrons or protons, interact and their spins are in a maximally entangled singlet state $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ afterwards. Then both particles fly off in different directions freely while the spins remain in the singlet state. Subsequently σ_z spin measurements are performed on both particles.
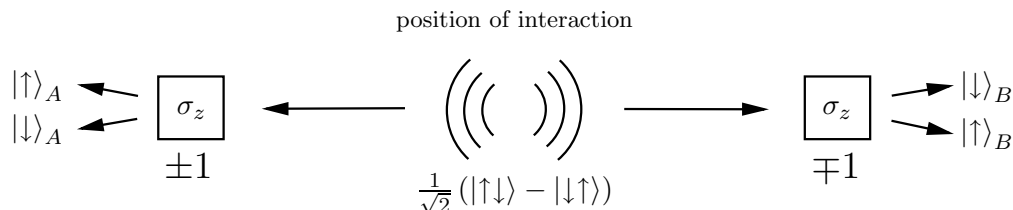

Figure 2.1: Schematic illustration of the Bohm-EPR situation

According to the measurement postulate of quantum mechanics the spin will no longer be a superposition of up $|\uparrow\rangle$ and down $|\downarrow\rangle$ though either one **or** the other. The reduction of the state vector to one of the eigenvectors of the observable σ_z of one particle forces the other particle's spin σ_z to be anti-correlated. Here appears a new type of simultaneousness. The problem here is that if one measures σ_z on one

side, the particle's spin on the other side is affected instantaneously, irrespective of how far they are apart. If the wave function is regarded as a real physical object this means that causality is violated, since one particle affects the other with superluminal velocity. When we say the measurements A and B are performed simultaneously then according to relativity there are different inertial frames of reference, in which A happens before B and vice versa. Fact is, quantum mechanics predicts that the spins are always perfectly anticorrelated. This phenomenon can be interpreted in different ways. When we accept the wave function as a real existing physical object we have to reject locality, since the reduction of the wave function is a non-local process. In the conventional version of the Copenhagen interpretation where the wave function is not a physical object of reality but rather a mathematical tool, realism is rejected in order to preserve locality[4]. In the Bohm interpretation locality is given up to maintain realism. What can be concluded from those interpretations is that, if nature really behaves quantum mechanically, then it is not local **and** realistic at the same time.

2.2 A Bell inequality for two-qubit systems: CHSH

As previously mentioned, local realistic theories are in contradiction to quantum mechanics in certain experiments. In order to show this, we derive a **Bell inequality** which holds for any local realistic theory but can be violated by quantum mechanics. This will be the famous **Clauser-Horne-Shimony-Holt inequality (CHSH)**, which is a modification of the original Bell inequality permitting experimental revisal.

2.2.1 Derivation of the CHSH inequality

We want to describe the Bohm-EPR situation with a local realistic theory. In order to do this, we introduce the parameter λ, which represents a hidden variable or a set of those. The spin of a particle then depends on the measured direction represented by a vector $\vec{a}$ and the parameter λ. We know that a spin measurement on a particle has only two possible outcomes. Without loss of generality we assign the values $+1$ and -1 to them. In a local realistic theory the observables of distant parties are then given by

$$A(\vec{a}, \lambda) = \pm 1 \ , \tag{2.1}$$

with measurement direction $\vec{a}$ on Alice's side, and

$$B(\vec{b}, \lambda) = \pm 1 \ , \tag{2.2}$$

with measurement direction $\vec{b}$ on Bob's side. Locality requires that the outcome of A does not depend on $\vec{b}$ and B does not depend on $\vec{a}$. Without loss of generality we can say that the value λ is achieved with probability density $\rho(\lambda) \geq 0$ obeying

$$\int \rho(\lambda) d\lambda = 1 \ . \tag{2.3}$$

---

[4]"There is no quantum world. There is only an abstract physical description. It is wrong to think that the task of physics is to find out how nature is. Physics concerns what we can say about nature." - Niels Bohr

We define a correlation function for the joint spin measurement, that yields the value 1 when the spins are parallel and -1 when the they are antiparallel

$$C\left(A(\vec{a},\lambda),B(\vec{b},\lambda)\right) = A(\vec{a},\lambda)\cdot B(\vec{b},\lambda) \ . \tag{2.4}$$

The expectation value of this quantity therefore is

$$E(\vec{a},\vec{b}) = \int \rho(\lambda)A(\vec{a},\lambda)B(\vec{b},\lambda)d\lambda \ . \tag{2.5}$$

If we combine different expectation values of different measurement directions in the following way

$$\begin{aligned}
E(\vec{a},\vec{b}) - E(\vec{a},\vec{b'}) &= \int \rho(\lambda)\left[A(\vec{a},\lambda)B(\vec{b},\lambda) - A(\vec{a},\lambda)B(\vec{b'},\lambda)\right]d\lambda \\
&= \int \rho(\lambda)A(\vec{a},\lambda)B(\vec{b},\lambda)\left[1 \pm A(\vec{a'},\lambda)B(\vec{b'},\lambda)\right]d\lambda \\
&\quad - \int \rho(\lambda)A(\vec{a},\lambda)B(\vec{b'},\lambda)\left[1 \pm A(\vec{a'},\lambda)B(\vec{b},\lambda)\right]d\lambda \ , \tag{2.6}
\end{aligned}$$

then the absolute value yields

$$\begin{aligned}
|E(\vec{a},\vec{b}) - E(\vec{a},\vec{b'})| &\leq \left|\int \rho(\lambda)\left[1 \pm A(\vec{a'},\lambda)B(\vec{b'},\lambda)\right]d\lambda\right| \\
&\quad + \left|\int \rho(\lambda)\left[1 \pm A(\vec{a'},\lambda)B(\vec{b},\lambda)\right]d\lambda\right| \\
&= 2 \pm |E(\vec{a'},\vec{b'}) + E(\vec{a'},\vec{b})| \ . \tag{2.7}
\end{aligned}$$

We obtain the **CHSH inequality** by rewriting this in the form

$$|E(\vec{a},\vec{b}) - E(\vec{a},\vec{b'}) + E(\vec{a'},\vec{b'}) + E(\vec{a'},\vec{b})| \leq 2 \ . \tag{2.8}$$

The derivation reveals that every local realistic theory has to fulfill the CHSH inequality. Quantum mechanics however predicts a violation under particular circumstances. Consider the quantum mechanical expectation value of $E(\vec{a},\vec{b})$ for the Bell state $|\Psi^-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

$$E(\vec{a},\vec{b}) = \left\langle \Psi^- \right| \vec{a}\cdot\vec{\sigma} \otimes \vec{b}\cdot\vec{\sigma} \left| \Psi^- \right\rangle \ , \tag{2.9}$$

with unit vectors $\vec{a}$ and $\vec{b}$. A short evaluation yields

$$E(\vec{a},\vec{b}) = -\vec{a}\cdot\vec{b} = -cos(\alpha - \beta) \ , \tag{2.10}$$

wherein the angles α and β substitute the vectors $\vec{a}$ and $\vec{b}$. Hence, we can write the CHSH inequality in the form

$$|-cos(\alpha - \beta) + cos(\alpha - \beta') - cos(\alpha' - \beta) - cos(\alpha' - \beta')| \ , \tag{2.11}$$

wherein α, α', β and β' are the angles of the four vectors $\vec{a}, \vec{a'}, \vec{b}$ and $\vec{b'}$ in a plane. For angles obeying $|\alpha - \beta| = |\alpha' - \beta| = |\alpha' - \beta'| = \frac{\pi}{4}$ and $|\alpha - \beta'| = \frac{3\pi}{4}$ we find

$$\begin{aligned}
|-cos(\alpha - \beta) &+ cos(\alpha - \beta') - cos(\alpha' - \beta) - cos(\alpha' - \beta')| \\
&= |-\frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2}| = 2\sqrt{2} > 2 \ . \tag{2.12}
\end{aligned}$$

As a result we have found that any local realistic theory cannot reproduce the statistics of quantum mechanics. Experiments with entangled photons confirm the violation of the CHSH inequality (see [2], [32]).

2.2.2 Horodecki violation criterion

The example with the singlet state $|\Psi^-\rangle$ demonstrates the violation of the CHSH inequality. Now we want to work out the whole set of states causing violations. For an arbitrary mixed state ρ the expectation value $E(\vec{a}, \vec{b})$ is

$$E(\vec{a}, \vec{b}) = Tr(\rho\, \vec{a} \cdot \vec{\sigma} \otimes \vec{b} \cdot \vec{\sigma})\,. \tag{2.13}$$

Thus, we can write the Bell inequality in the form

$$\left| Tr\left(\rho\left[\vec{a} \cdot \vec{\sigma} \otimes (\vec{b} - \vec{b'}) \cdot \vec{\sigma} + \vec{a'} \cdot \vec{\sigma} \otimes (\vec{b} + \vec{b'}) \cdot \vec{\sigma}\right]\right)\right| \le 2\,. \tag{2.14}$$

We call the operator in square brackets the **Bell operator** $\mathcal{B}$

$$\mathcal{B}(\vec{a}, \vec{a'}, \vec{b}, \vec{b'}) = \vec{a} \cdot \vec{\sigma} \otimes (\vec{b} - \vec{b'}) \cdot \sigma + \vec{a'} \cdot \vec{\sigma} \otimes (\vec{b} + \vec{b'}) \cdot \vec{\sigma}\,. \tag{2.15}$$

It is obvious that for a given state ρ one has to find the right vectors $\vec{a}, \vec{a'}, \vec{b}$ and $\vec{b'}$ to show possible violation. Only if the global maximum with respect to all Bell operators $\mathcal{B}(\vec{a}, \vec{a'}, \vec{b}, \vec{b'})$ is less or equal to 2, then the inequality is preserved

$$\max_{\vec{a}, \vec{a'}, \vec{b}, \vec{b'}} \left| Tr\left(\rho\left[\vec{a} \cdot \vec{\sigma} \otimes (\vec{b} - \vec{b'}) \cdot \vec{\sigma} + \vec{a'} \cdot \vec{\sigma} \otimes (\vec{b} + \vec{b'}) \cdot \vec{\sigma}\right]\right)\right| \le 2\,. \tag{2.16}$$

Since the Bell operator $\mathcal{B}(\vec{a}, \vec{a'}, \vec{b}, \vec{b'})$ is expressed in terms of Pauli matrices, it makes sense to express ρ in the way we introduced it in (1.16)

$$\rho = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + \vec{r} \cdot \vec{\sigma} \otimes \mathbb{1} + \mathbb{1} \otimes \vec{s} \cdot \vec{\sigma} + \sum_{n,m=1}^{3} t_{nm}\sigma_n \otimes \sigma_m\right)\,. \tag{2.17}$$

The computation of $|Tr(\rho\mathcal{B})|$ then yields

$$\left| \vec{a} \cdot T(\rho)(\vec{b} - \vec{b'}) + \vec{a'} \cdot T(\rho)(\vec{b} + \vec{b'})\right|\,, \tag{2.18}$$

wherein $T(\rho)$ denotes the 3×3 correlation matrix with the coefficients t_{nm}. We replace $\vec{b} - \vec{b'}$ and $\vec{b} + \vec{b'}$ by mutually orthogonal unit vectors $\vec{c}$ and $\vec{c'}$

$$\vec{b} - \vec{b'} = 2\sin\theta\vec{c'} \qquad \vec{b} + \vec{b'} = 2\cos\theta\vec{c}\,. \tag{2.19}$$

Now the maximum of $|Tr(\rho\mathcal{B})|$ has to be determined with respect to $\theta, \vec{a}, \vec{a'}, \vec{c}$ and $\vec{c'}$

$$\max_{\theta, \vec{a}, \vec{a'}, \vec{c}, \vec{c'}} 2\left|\sin\theta\vec{a} \cdot T(\rho)\vec{c'} + \cos\theta\vec{a'} \cdot T(\rho)\vec{c}\right|\,. \tag{2.20}$$

The scalar products are maximal for parallel vectors. Consequently, we choose the unit vectors $\vec{a}_{max} = \frac{T(\rho)\vec{c'}}{\|T(\rho)\vec{c'}\|}$ and $\vec{a'}_{max} = \frac{T(\rho)\vec{c}}{\|T(\rho)\vec{c}\|}$

$$\max_{\theta, \vec{c}, \vec{c'}} 2\left|\sin\theta\|T(\rho)\vec{c'}\| + \cos\theta\|T(\rho)\vec{c}\|\right|\,. \tag{2.21}$$

Maximisation with respect to θ yields

$$\max_{\vec{c}, \vec{c'}} 2\sqrt{\|T(\rho)\vec{c'}\|^2 + \|T(\rho)\vec{c}\|^2}\,. \tag{2.22}$$

Since $\vec{c}$ and $\vec{c'}$ are mutually orthogonal unit vectors, the expressions $\|T(\rho)\vec{c'}\|^2 = \vec{c'} \cdot T^T(\rho)T(\rho)\vec{c'}$ and $\|T_\rho\vec{c}\|^2 = \vec{c}\cdot T^T(\rho)T(\rho)\vec{c}$ are maximal when $\vec{c'}$ and $\vec{c}$ are eigenvectors of the two largest eigenvalues $\lambda_1(\rho)$ and $\lambda_2(\rho)$ of $K(\rho) = T^T(\rho)T(\rho)$. Thus the CHSH inequality reads

$$2\sqrt{\lambda_1(\rho) + \lambda_2(\rho)} \le 2 \ . \tag{2.23}$$

Now we have proven that if and only if the two largest eigenvalues of the matrix $K(\rho) = T^T(\rho)T(\rho)$ comply

$$\lambda_1(\rho) + \lambda_2(\rho) > 1 \ , \tag{2.24}$$

then the state ρ violates the CHSH inequality for particular vectors $\vec{a}, \vec{a'}, \vec{b}$ and $\vec{b'}$. This necessary and sufficient condition was found by the Horodeckis in 1995 [33].

2.3 A Bell inequality for bipartite qudit systems: CGLMP

The CHSH inequality is a Bell inequality for bipartite qubit systems. In this section we present Bell inequalities for bipartite qudit systems based on logical constraints established by Collins, Gisin, Linden, Massar and Popescu (**CGLMP**)[34] .

2.3.1 Derivation of the CGLMP inequality

Once again, we consider the standard situation with the two parties Alice and Bob spatially separated, only having access onto their local Hilbert spaces $\mathcal{H}^A = \mathcal{H}^B = \mathbb{C}^d$ of dimension d, while the composite Hilbert space is once again $\mathcal{H}^{AB} = \mathbb{C}^d \otimes \mathbb{C}^d$. Consequently, measurements on each side have d possible outcomes. Let us assume again that we could reproduce the statistical predictions with a local realistic theory. In analogy to the CHSH Bell experiment, each party has two apparatuses with different settings. Due to the fact that in a local realistic theory all observables have definite values simultaneously, the state of a system induces a probability distribution of form

$$P(A_1 = j, A_2 = k, B_1 = l, B_2 = m) \tag{2.25}$$

that apparatus A_1 gives measurement result $j \in \{0, .., d-1\}$, apparatus A_2 gives $k \in \{0, .., d-1\}$ and so on. In sum, we have d^4 values determining the statistics of the system. As usual we normalise these probabilities

$$\sum_{jklm} P(A_1 = j, A_2 = k, B_1 = l, B_2 = m) = 1 \ . \tag{2.26}$$

If we are only interested in measurement results of certain apparatuses then we have to sum over all ignored observables. For example the probability of A_1 giving j and B_1 giving l is $P(A_1 = j, B_1 = l) = \sum_{km} P(A_1 = j, A_2 = k, B_1 = l, B_2 = m)$. We introduce some variables r', s', t' and u' defined by relations of measurement outcomes

$$r' = B_1 - A_1 = l - j \ , \tag{2.27}$$
$$s' = A_2 - B_1 = k - l \ , \tag{2.28}$$
$$t' = B_2 - A_2 = m - k \ , \tag{2.29}$$
$$u' = A_1 - B_2 = j - m \ . \tag{2.30}$$

The definition induces the constraint

$$(r' + s' + t' + u') \bmod d = 0 \ . \tag{2.31}$$

We introduce the quantity I defined by

$$I = P(A_1 = B_1) + P(B_1 = A_2 + 1) + P(A_2 = B_2) + P(B_2 = A_1) \ , \tag{2.32}$$

with the probabilities $P(A_a = B_b + k)$ that the outcome of A_a differs from outcome B_b by k

$$P(A_a = B_b + k) = \sum_{j=0}^{d-1} P(A_a = (j + k) \bmod d, B_b = j) \ . \tag{2.33}$$

Then I is the sum of the probabilities that $r' = 0, s' = -1, t' = 0$ and $u' = 0$. Nevertheless, because of the logical constraint $r' + s' + t' + u' = 0$ only three of those four relations can be valid. Thus we have

$$I \leq 3 \tag{2.34}$$

for all local realistic theories. We introduce another quantity I_3

$$\begin{aligned}
I_3 = &+ [P(A_1 = B_1) + P(B_1 = A_2 + 1) + P(A_2 = B_2) + P(B_2 = A_1)] \tag{2.35}\\
&- [P(A_1 = B_1 - 1) + P(B_1 = A_2) + P(A_2 = B_2 - 1) + P(B_2 = A_1 - 1)]
\end{aligned}$$

Consider the following table which shows how the logical constraint affects the maximum of I_3.

+1				-1				
r'	s'	t'	u'	r'	s'	t'	u'	
0	-1	0	0	1	0	1	1	
	◆	◆	◆	◆				$\Rightarrow I_3 = 2$
◆		◆	◆		◆			$\Rightarrow I_3 = 2$
◆	◆		◆			◆		$\Rightarrow I_3 = 2$
◆	◆	◆					◆	$\Rightarrow I_3 = 2$

In consequence

$$I_3 \leq 2. \tag{2.36}$$

Additional quantities I_d can be introduced[5]

$$\begin{aligned}
I_d = \sum_{k=0}^{[d/2]-1} \left(1 - \frac{2k}{d-1}\right)\Big\{ &+ \big[P(A_1 = B_1 + k) + P(B_1 = A_2 + k + 1) \tag{2.37}\\
&+ P(A_2 = B_2 + k) + P(B_2 = A_1 + k)\big]\\
&- \big[P(A_1 = B_1 - k - 1) + P(B_1 = A_2 - k)\\
&+ P(A_2 = B_2 - k - 1) + P(B_2 = A_1 - k - 1)\big]\Big\}
\end{aligned}$$

For local realistic theories the upper bound is 2

$$I_d \leq 2 \ . \tag{2.38}$$

---

[5] the bracket [ ] stands for the floor function

Proof: We introduce the variables

$$r = A_1 - B_1 \ , \tag{2.39}$$
$$s = B_1 - A_2 - 1 \ , \tag{2.40}$$
$$t = A_2 - B_2 \ , \tag{2.41}$$
$$u = B_2 - A_1 \ , \tag{2.42}$$

that obey

$$(r + s + t + u + 1) \bmod d = 0 \ . \tag{2.43}$$

Since all computations are done modulo d, without loss of generality we can restrict r, s, t and u to lie in the interval

$$-[\frac{d}{2}] \leq r, s, t, u \leq [\frac{(d-1)}{2}] \ . \tag{2.44}$$

I_d can be written as a function depending on r, s, t and u in the following way

$$I_d = f(r) + f(s) + f(t) + f(u) \ , \tag{2.45}$$

where $f(x)$ is given by

$$f(x) = \begin{cases} \dfrac{-2x}{d-1} + 1 & x \geq 0 \\ \dfrac{-2x}{d-1} - \dfrac{d+1}{d-1} & x < 0 \ . \end{cases} \tag{2.46}$$

We now have to check all combinations of algebraic signs of r, s, t and u. With help of (2.43) and (2.44) we find

- $r, s, t, u \geq 0$:
  $\Rightarrow r + s + t + u + 1 = d \Rightarrow I_d = 2$

- three of r, s, t, u are ≥ 0 and one is < 0 :
  either $r + s + t + u + 1 = d \Rightarrow I_d = 2$
  or $r + s + t + u + 1 = 0 \Rightarrow I_d = \frac{-2}{d-1}$

- two of r, s, t, u are ≥ 0 and two are < 0 :
  $\Rightarrow r + s + t + u + 1 = 0 \Rightarrow I_d = \frac{-2}{d-1}$

- one of r, s, t, u is ≥ 0 and three are < 0 :
  either $r + s + t + u + 1 = 0 \Rightarrow I_d = \frac{-2(d+1)}{d-1}$
  or $r + s + t + u + 1 = -d \Rightarrow I_d = \frac{-2}{d-1}$

- $r, s, t, u < 0$:
  $\Rightarrow r + s + t + u + 1 = -d \Rightarrow I_d = \frac{-2(d+1)}{d-1}$

Hence, $I_d \leq 2$. $\square$

In the following, we investigate the predictions of quantum mechanics for this family of inequalities. First, we have to insert the quantum mechanical probabilities

$$P(A_a = k, B_b = l) = Tr\left(\rho\,|k\rangle_{Aa}\,\langle k|_{Aa} \otimes |l\rangle_{Bb}\,\langle l|_{Bb}\right)\;, \tag{2.47}$$

wherein $\{|k\rangle_{Aa}\}$ and $\{|l\rangle_{Bb}\}$ denote orthonormal eigenvectors of the observables with $k, l \in \{0, .., d-1\}$. To confirm the violation of these inequalities consider the maximally entangled state

$$|\Omega_{0,0}\rangle = \frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} |s\rangle_A \otimes |s\rangle_B \tag{2.48}$$

and orthonormal eigenvectors

$$|k\rangle_{Aa} = \frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} \exp\left(\frac{2\pi i}{d} s(k + \alpha_a)\right) |s\rangle_A\;, \tag{2.49}$$

$$|l\rangle_{Bb} = \frac{1}{\sqrt{d}} \sum_{s=0}^{d-1} \exp\left(\frac{2\pi i}{d} s(-l + \beta_b)\right) |s\rangle_B\;, \tag{2.50}$$

with $\alpha_1 = 0$, $\alpha_2 = \frac{1}{2}$, $\beta_1 = \frac{1}{4}$ and $\beta_2 = -\frac{1}{4}$. Then (2.47) becomes

$$
\begin{aligned}
&P(A_a = k, B_b = l)\\
=&Tr\left(|\Omega_{0,0}\rangle\,\langle\Omega_{0,0}|\,|k\rangle_{Aa}\,\langle k|_{Aa} \otimes |l\rangle_{Bb}\,\langle l|_{Bb}\right)\\
=&\left|\langle\Omega_{0,0}|\,|k\rangle_{Aa} \otimes |l\rangle_{Bb}\right|^2\\
=&\frac{1}{d^2}\left|\langle\Omega_{0,0}|\left[\sum_{r=0}^{d-1}\exp\left(\frac{2\pi i}{d}r(k+\alpha_a)\right)|r\rangle_A\right] \otimes \left[\sum_{m=0}^{d-1}\exp\left(\frac{2\pi i}{d}m(-l+\beta_b)\right)|m\rangle_A\right]\right|^2\\
=&\frac{1}{d^3}\left|\sum_{s,r,m=0}^{d-1}\underbrace{\langle s|_A|r\rangle_A}_{\delta_{sr}}\underbrace{\langle s|_B|m\rangle_B}_{\delta_{sm}}\exp\left(\frac{2\pi i}{d}r(k+\alpha_a)\right)\exp\left(\frac{2\pi i}{d}m(-l+\beta_b)\right)\right|^2\\
=&\frac{1}{d^3}\left|\sum_{s=0}^{d-1}\exp\left(\frac{2\pi i}{d}s(k-l+\alpha_a+\beta_b)\right)\right|^2\\
=&\frac{\sin^2\left(\pi(k-l+\alpha_a+\beta_b)\right)}{d^3\sin^2\left(\pi(k-l+\alpha_a+\beta_b/d)\right)}\;.
\end{aligned}
\tag{2.51}
$$

With the values of α_1, α_2, β_1 and β_2 given above we find

$$P(A_a = k, B_b = l) = \frac{1}{2d^3\sin^2\left(\pi(k-l+\alpha_a+\beta_b)/d\right)}\;. \tag{2.52}$$

Inserting this into I and I_d leads to

$$I = \frac{2}{d^2\sin^2\left(\frac{\pi}{4d}\right)}\;, \tag{2.53}$$

$$I_d = \frac{2}{d^2}\sum_{k=0}^{\left[\frac{d}{2}\right]-1}\left(1 - \frac{2k}{d-1}\right)\left(\frac{1}{\sin^2\left(\frac{\pi}{d}(k+\frac{1}{4})\right)} - \frac{1}{\sin^2\left(\frac{-\pi}{d}(k+\frac{3}{4})\right)}\right)\;. \tag{2.54}$$

We obtain the following values for I and I_d

d	2	3	4	5	6	7		$\rightarrow \infty$
I	3.41421	3.31738	3.28427	3.26908	3.26086	3.25592		3.24228
violation [%]	13.8071	10.5793	9.47559	8.96922	8.69533	8.53059		8.07593
I_d	2.82843	2.87293	2.89624	2.91054	2.92020	2.92716		2.96981
violation [%]	41.4214	43.6467	44.8122	45.5272	46.0102	46.358		48.4906

As we can see, the **CGLMP inequalities** $I \leq 3$ and $I_d \leq 2$ are violated. The table also reveals that by using I_d instead of I we achieve much stronger violations. This is in close relation to the resistance against noise. Before we analyse this, we present a concise notation for I and I_d. Due to (2.47) the probabilities $P(A_a = B_b + k)$ become

$$P(A_a = B_b + k) = \sum_{j=0}^{d-1} Tr\left(\rho \left|(j+k) \bmod d\right\rangle_{Aa} \left\langle(j+k) \bmod d\right|_{Aa} \otimes |j\rangle_{Bb} \langle j|_{Bb}\right) .$$

We rewrite I by exploiting linearity of the trace in the following way

$$I = P(A_1 = B_1) + P(A_2 = B_2) + P(B_1 = A_2 + 1) + P(B_2 = A_1)$$

$$= Tr\left(\rho \sum_{j=0}^{d-1} \Big\{ |j\rangle_{A1} \langle j|_{A1} \otimes |j\rangle_{B1} \langle j|_{B1} + |j\rangle_{A2} \langle j|_{A2} \otimes |j\rangle_{B2} \langle j|_{B2}\right.$$

$$\left. + |(j-1) \bmod d\rangle_{A2} \langle(j-1) \bmod d|_{A2} \otimes |j\rangle_{B1} \langle j|_{B1} + |j\rangle_{A1} \langle j|_{A1} \otimes |j\rangle_{B2} \langle j|_{B2} \Big\}\right)$$

$$= Tr\left(\rho \mathcal{B}_I\right) . \tag{2.55}$$

We identify the sum of operators as our new **Bell operator** $\mathcal{B}_I$ for I. In the same way we can define Bell operators $\mathcal{B}_{I_d}$ for all quantities I_d so that

$$I_d = Tr\left(\rho \mathcal{B}_{I_d}\right) . \tag{2.56}$$

Now, let us consider the state $|\Omega_{0,0}\rangle$ in presence of uncolored noise

$$\rho = (1-r) |\Omega_{0,0}\rangle \langle\Omega_{0,0}| + r\frac{\mathbb{1}}{d^2} , \tag{2.57}$$

wherein $r \in [0,1]$ is the amount of noise. We obtain

$$I = Tr\left(\rho \mathcal{B}_I\right) = (1-r)Tr\left(|\Omega_{0,0}\rangle \langle\Omega_{0,0}| \mathcal{B}_I\right) + \frac{r}{d^2} Tr\mathcal{B}_I , \tag{2.58}$$

$$I_d = Tr\left(\rho \mathcal{B}_{I_d}\right) = (1-r)Tr\left(|\Omega_{0,0}\rangle \langle\Omega_{0,0}| \mathcal{B}_{I_d}\right) + \frac{r}{d^2} Tr\mathcal{B}_{I_d} . \tag{2.59}$$

$\mathcal{B}_I$ contains $4d$ projectors with prefactor 1, hence $Tr\mathcal{B}_I = 4d$. Whereas the addends in $\mathcal{B}_{I_d}$ contain $4d$ projectors with prefactor $\left(1 - \frac{2k}{d-1}\right)$ and $4d$ projectors with prefactor $-\left(1 - \frac{2k}{d-1}\right)$, hence $Tr\mathcal{B}_{I_d} = 0$. In consequence, we obtain

$$I = (1-r)Tr\left(|\Omega_{0,0}\rangle \langle\Omega_{0,0}| \mathcal{B}_I\right) + r\frac{4}{d} , \tag{2.60}$$

$$I_d = (1-r)Tr\left(|\Omega_{0,0}\rangle \langle\Omega_{0,0}| \mathcal{B}_{I_d}\right) . \tag{2.61}$$

Above a certain amount of noise $r = r_{max}$, the state ρ ceases to violate the Bell inequality. The values are given by $I(r_{max}) = 3$ and $I_d(r_{max}) = 2$, and are summarised in the following table.

d	2	3	4	5	6	7		$\to \infty$
$I : r_{max}$ [%]	29.2893	15.9965	12.4446	10.8979	10.0555	9.5332		7.47246
$I_d : r_{max}$ [%]	29.2893	30.3848	30.9450	31.2843	31.5116	31.6744		32.6557

We conclude that one should give preference to the inequalities $I_d \leq 2$ due to their higher resistance to noise.

2.3.2 Optimisation of the Bell operator

The orthonormal bases given in (2.49) are optimal for the state $|\Omega_{0,0}\rangle$. In other words, there exists no better Bell operator for $|\Omega_{0,0}\rangle$ causing higher violation. This has not been proven so far, though numerical optimisation indicates that this is true (see [34],[35]). The lack of a proof lies in the fact that the finding of an optimal Bell operator for an arbitrary ρ is a nonlinear optimisation problem: The finding of solutions for $\mathrm{grad}(Tr(\rho\mathcal{B})) = 0$ with respect to all vector components is a nonlinear task and is further complicated by nonlinear constraints since the vectors $\{|k\rangle_{Aa}\}$ and $\{|l\rangle_{Bb}\}$ have to form an orthonormal basis (observables are hermitian operators and their eigenvectors are orthogonal)

$$\langle k|_{Aa} |j\rangle_{Aa} = \delta_{kj} \ , \tag{2.62}$$

$$\langle l|_{Bb} |m\rangle_{Bb} = \delta_{lm} \ . \tag{2.63}$$

Using the Weyl operators or the Gell-Mann matrices to express ρ and $\mathcal{B}$ does not lead to a simplification like in §2.2.2 for the CHSH inequality. For this reason, we have developed a numerical optimisation algorithm which reliably finds optimal Bell operators for any ρ. Let us first investigate the number of variables of the Bell operator $\mathcal{B}$. We have 4 orthonormal bases $\{|k\rangle_{A1}\}, \{|k\rangle_{A2}\}, \{|l\rangle_{B1}\}$ and $\{|l\rangle_{B2}\}$ with each d vectors. Each vector is an element of $\mathbb{C}^d$ and can be described by 2d real numbers (d vector components, each described by 2 real numbers, one for the amplitude and one for the phase). Altogether we have $4 \times d \times 2d = 8d^2$ real variables. Orthonormality restricts the values of the variables, thus we have to optimise $\mathcal{B}$ under the constraints (2.62) and (2.63). For all practical purposes however this way is quite impractical. We now show how to satisfy the constraints by choosing the right set of variables. We begin with some mathematical considerations. Any basis transformation can be realised via a unitary transformation, i.e. any basis $\{|k\rangle\}$ of $\mathbb{C}^d$ can be transformed into any other basis $\{|k'\rangle\}$ of $\mathbb{C}^d$ by means of a certain unitary transformation $\{|k'\rangle\} = \{U|k\rangle\}$. Since it is our goal to find the right orthonormal bases $\{|k\rangle_{A1}\}, \{|k\rangle_{A2}\}, \{|l\rangle_{B1}\}$ and $\{|l\rangle_{B2}\}$, we can select arbitrary orthonormal bases and seek the unitary transformations U_{A1}, U_{A2}, U_{B1} and U_{B1} that maximise I_d and I. These transformations are elements of the unitary group $U(d)$. Due to the fact that global phases do not affect probabilities and that $U(d)$ can be written as a semidirect product $U(d) \cong SU(d) \times U(1)$, it suffices to regard the special unitary group $SU(d)$. We use the **generalised Euler angle parametrisation** of this group, wherein the Euler angles embody all degrees of freedom (see [36],[37]). For this kind of parametrisation the following antisymmetric and diagonal generalised

Gell-Mann matrices (1.38,1.39) are needed

$$\lambda_{k^2-1} \equiv \Lambda^{k-2} = \sqrt{\frac{2}{(k-1)k}} \left(\sum_{j=0}^{k-2} |j\rangle \langle j| - (k-1) |k-1\rangle \langle k-1| \right) \qquad 2 \le k \le d \ ,$$

$$\lambda_{k^2+1} \equiv \Lambda_a^{0k} = -i |0\rangle \langle k| + i |k\rangle \langle 0| \qquad\qquad 1 \le k \le d-1 \ .$$

In this notation the explicit form of the parametrisation of $U \in SU(d)$ by generalised Euler angles $\{\alpha_i\}$ reads (see [36], [37][6])

$$U = \left[\prod_{x=0}^{d-2} \left(\prod_{k=2}^{d-x} A(k,j(x)) \right) \right] \left[\prod_{n=2}^{d} \exp(i\lambda_{n^2-1}\alpha_{d^2-(d+1-n)}) \right] \ , \qquad (2.64)$$

with $A(k,j(x))$ and $j(x)$ given by

$$A(k,j(x)) = \exp(i\lambda_3\alpha_{(2k-3)+j(x)}) \cdot \exp(i\lambda_{(k-1)^2+1}\alpha_{2(k-1)+j(m)}) \ , \qquad (2.65)$$

$$j(x) = \begin{cases} 0 & x = 0 \\ 2\sum_{l=0}^{x-1}(d-x+l) & x > 0 \ . \end{cases} \qquad (2.66)$$

For instance, for $d = 2, 3, 4$ we find

$$U \in SU(2) \Longleftrightarrow U = \exp(i\lambda_3\alpha_1) \cdot \exp(i\lambda_2\alpha_2) \cdot \exp(i\lambda_3\alpha_3) \ , \qquad (2.67)$$

$$\begin{aligned} U \in SU(3) \Longleftrightarrow U = {} & \exp(i\lambda_3\alpha_1) \cdot \exp(i\lambda_2\alpha_2) \cdot \exp(i\lambda_3\alpha_3) \cdot \exp(i\lambda_5\alpha_4) \\ & \cdot \exp(i\lambda_3\alpha_5) \cdot \exp(i\lambda_2\alpha_6) \cdot \exp(i\lambda_3\alpha_7) \cdot \exp(i\lambda_8\alpha_8) \ , \end{aligned} \qquad (2.68)$$

$$\begin{aligned} U \in SU(4) \Longleftrightarrow U = {} & \exp(i\lambda_3\alpha_1) \cdot \exp(i\lambda_2\alpha_2) \cdot \exp(i\lambda_3\alpha_3) \cdot \exp(i\lambda_5\alpha_4) \\ & \cdot \exp(i\lambda_3\alpha_5) \cdot \exp(i\lambda_{10}\alpha_6) \cdot \exp(i\lambda_3\alpha_7) \cdot \exp(i\lambda_2\alpha_8) \\ & \cdot \exp(i\lambda_3\alpha_9) \cdot \exp(i\lambda_5\alpha_{10}) \cdot \exp(i\lambda_3\alpha_{11}) \cdot \exp(i\lambda_2\alpha_{12}) \\ & \cdot \exp(i\lambda_3\alpha_{13}) \cdot \exp(i\lambda_8\alpha_{14}) \cdot \exp(i\lambda_{15}\alpha_{15}) \ . \end{aligned} \qquad (2.69)$$

The parametrisation guarantees compliance with the constraints (2.62) and (2.63) and reduces the number of variables to $4(d^2 - 1)$ without discarding any solution. However, the optimisation of $\mathcal{B}$ with respect to the Euler angles still requires a numerical optimisation algorithm. While popular algorithms like **Differential Evolution**, **Simulated Annealing** or **gradient based methods** have been very time-consuming, the **Nelder-Mead method** [38] has performed this task relatively fast and reliable. In general this method can be advantageous when the number of variables is very large, because it manages to find a maximum without computing derivatives, which can possibly be computationally intensive. For maximisation the algorithm proceeds as follows: Assume a function $f(x_1, .., x_n)$ which has to be maximised with respect to n variables $y = (x_1, .., x_n)$. At the beginning a simplex with $n + 1$ vertices $y_1, .., y_{n+1}$ is created at random. In the first step (1) the vertices are being arranged by their values $f(y)$ and labeled according to

$$f(y_1) \ge f(y_2) \ge \ldots \ge f(y_{n+1}) \ . \qquad (2.70)$$

---

[6]Note that our notation differs slightly. We chose an indexing where all indices are increasing and the sequence of the product is $\prod_{i=1}^{N} A_i = A_1 \cdot A_2 \cdots A_N$

According to this, $f(y_1)$ is the best and $f(y_{n+1})$ the worst vertex. Then a reflection of the worst point through the centroid of the remaining n points $y_0 = \frac{1}{n}\sum_{i=1}^{n} y_i$ is performed

$$y_r = y_0 + \alpha(y_0 - y_{n+1}) , \qquad (2.71)$$

where $\alpha > 0$ is called the reflection parameter. The next step of the procedure depends on the value $f(y_r)$:

- If $f(y_r)$ is better than $f(y_n)$ but not better than $f(y_1)$, i.e. $f(y_1) \geq f(y_r) > f(y_n)$ then a new simplex with y_{n+1} substituted by y_r is built and step (1) is repeated.

- If $f(y_r)$ is the best point, i.e. $f(y_r) > f(y_1)$ then an expansion $y_e = y_0 + \gamma(y_0 - y_{n+1})$ with expansion parameter $\gamma > 0$ is performed. If $f(y_e) > f(y_r)$ then a new simplex with y_{n+1} substituted by y_e is built and step (1) is repeated. Otherwise y_r is used instead of y_e.

- If $f(y_r)$ does not result in an improvement, i.e. $f(y_r) \leq f(y_{n+1})$ then a contraction $y_c = y_{n+1} + \rho(y_0 - y_{n+1})$ with contraction parameter $\rho > 0$ is performed. If $f(y_c) \geq f(y_{n+1})$, then a new simplex with y_{n+1} substituted by y_c is built and step (1) is repeated. Else the simplex is being shrinked: The vertices are being replaced by $y_1' = y_1$ and $y_i' = y_1 + \sigma(y_i - y_1)$ with shrink parameter $\sigma > 0$ for all $i \in \{2, .., n+1\}$, afterwards step (1) is repeated.

The rules are repeated until the convergence criteria $|f(y_1') - f(y_1)| < c_1$ and $\|y_1' - y_1\| < c_2$ are satisfied, where y_1' is the new and y_1 the old best point, and $c_1, c_2 > 0$ are constants depending on the desired precision. As we can infer from the rules, the Nelder-Mead method is a hill climbing algorithm, which has the disadvantage that it could converge at a local maximum. We cannot completely avoid this problem; however, by varying the starting points we will find the global maximum in all likelihood.

The optimisation procedures for the Bell operators $\mathcal{B}_{I_3}$ and $\mathcal{B}_{I_4}$ via the Euler angle parametrisation and the Nelder-Mead method have been realised in MATHEMATICA 6 and can be found in the appendix B and C. To achieve good results it was necessary to find proper values for the parameters α, γ, ρ and σ. With the values $\alpha = 1.6, \gamma = 1.6, \rho = 0.8$ and $\sigma = 0.8$ an agreeable compromise between robustness against local maxima and time exposure was attained (with the standard values the algorithm converges at local maxima more often). We have chosen to execute the algorithm ten times with different starting simplices to guarantee that the global maximum is obtained. The accuracy/precision goal has been set to MATHEMATICA 6 standard values $c_1 = c_2 = 10^{-8}$.

2.3.3 Properties

Before we discuss some properties of the CGLMP inequalities we show that the inequality $I_d \leq 2$ is equivalent to the CHSH inequality when the regarded Hilbert space is two dimensional $\mathcal{H}^A = \mathcal{H}^B = \mathbb{C}^2$. Correspondingly, all properties of the CGLMP inequalities $I_d \leq 2$ likewise hold for the CHSH inequality.

The proof of equivalence is straight forward. We write all terms of I_2 explicitly

$$
\begin{aligned}
I_2 = &+ [P(A_1 = B_1) + P(B_1 = A_2 + 1) + P(A_2 = B_2) + P(B_2 = A_1)] \\
&- [P(A_1 = B_1 - 1) + P(B_1 = A_2) + P(A_2 = B_2 - 1) + P(B_2 = A_1 - 1)] \\
= &+ [P(A_1 = 0, B_1 = 0) + P(A_1 = 1, B_1 = 1) + P(A_2 = 0, B_1 = 1) \\
&+ P(A_2 = 1, B_1 = 0) + P(A_2 = 0, B_2 = 0) + P(A_2 = 1, B_2 = 1) \\
&+ P(A_1 = 0, B_2 = 0) + P(A_1 = 1, B_2 = 1)] \\
&- [P(A_1 = 0, B_1 = 1) + P(A_1 = 1, B_1 = 0) + P(A_2 = 0, B_1 = 0) \\
&+ P(A_2 = 1, B_1 = 1) + P(A_2 = 0, B_2 = 1) + P(A_2 = 1, B_2 = 0) \\
&+ P(A_1 = 0, B_2 = 1) + P(A_1 = 1, B_2 = 0)] \ .
\end{aligned}
$$

Since the expectation value (2.5) can be written as $E(A, B) = \int \rho(\lambda) A(\lambda) B(\lambda) d\lambda = P(A = 0, B = 0) + P(A = 1, B = 1) - P(A = 0, B = 1) - P(A = 1, B = 0)$ we can summarise the terms of I_2 and find

$$
I_2 = E(A_1, B_1) - E(A_2, B_1) + E(A_2, B_2) + E(A_1, B_2) \leq 2 \ . \tag{2.72}
$$

Due to the symmetry of positive and negative terms of I_2 for dimension two, the inequality $|I_2| \leq 2$ holds too. Hence, this is exactly the CHSH inequality with A and B interchanged (which makes no difference).

Now we quote some important properties: The CGLMP inequalities have been proven to be **tight Bell inequalities** (see [39]). For the understanding of this, we have to return to the probability distribution (2.25) on which the CGLMP inequalities are based on. As noted before, there are d^4 values determining the statistics of a local realistic theory. In contrast, in quantum mechanics we have probability distributions $P(A_a = k, B_b = l)$, with $k, l \in \{0, .., d-1\}$ for each of the four settings $(A_1 B_1), (A_1 B_2), (A_2 B_1)$ and $(A_2 B_2)$. As we have seen, those cannot be reproduced by summing over all unregarded observables of $P(A_1 = j, A_2 = k, B_1 = l, B_2 = m)$. To conclude, we only have d^2 probabilities for each setting and $4d^2$ in total. The quantum mechanical probability distributions are restricted by normalisation

$$
\sum_{k,l=0}^{d-1} P(A_a = k, B_b = l) = 1 \qquad a, b = 1, 2 \ , \tag{2.73}
$$

and the non-signaling condition (quantum mechanics cannot be used for superluminal communication)

$$
\sum_{l=0}^{d-1} P(A_a = k, B_1 = l) = \sum_{l=0}^{d-1} P(A_a = k, B_2 = l) \qquad a = 1, 2 \tag{2.74}
$$

(it is clear, that the same has to hold for A and B interchanged) .

What have we gained? The quantum mechanical probabilities can be specified by $4d^2$ values, which can be regarded as entries of a vector $\mathbf{P} \in \mathcal{R}^{4d^2}$. Due to the constraints, all physical relevant vectors lie in an affine space of dimension $4d^2 - 4d$ (see [39]). In this context, the normalisation coming from the local realistic description of the

system restricts a vector $\mathbf{P}$ to belong to the convex hull of d^4 vectors $\mathbf{G}_i \in \mathcal{R}^{4d^2}$

$$\sum_{j,k,k,m=0}^{d-1} P(A_1 = j, A_2 = k, B_1 = l, B_2 = m) = 1 \ , \qquad (2.75)$$

$$\Rightarrow \mathbf{P}_{LR} = \sum_{i=1}^{d^4} c_i \mathbf{G}_i \qquad c_i \geq 0 \text{ and } \sum_{i=1}^{d^4} c_i = 1 \ . \qquad (2.76)$$

The extremal points $\mathbf{G}_i \in \mathcal{R}^{4d^2}$ then are the generators of a convex polytope. Such a polytope can also be described by facets and their half-spaces. Facets induce inequalities of form

$$\mathbf{P} \in \text{conv}\left(\{\mathbf{G}_i\}\right) \Longleftrightarrow \mathbf{X}_i \cdot \mathbf{P} \leq x_i \qquad \forall i \in \{1, 2, .., n\} \ , \qquad (2.77)$$

where n is the necessary number of facets to define the polytope. Hence, with this set of inequalities we can determine all states that are in contradiction to local realism in an experiment with two apparatuses on each side. The problem involved is, that computing the facets of a high-dimensional polytope is a very difficult task that has only been completely solved for d=2 (see [40]). Let us now compare this approach with our well-known Bell inequalities. We know that all states that violate a Bell inequality do not belong to the convex hull of $\{\mathbf{G}_i\}$. However, states that fulfill a Bell inequality do not necessarily belong to it. This means that Bell inequalities define a region (half-space, sphere, polytope, etc.) that contains the convex polytope. The term **tight Bell inequality** is used if the boundary of the generated region at least partially coincides with at least one of the facets of the polytope. Hence, the inequalities (2.77) are themselves tight Bell inequalities as well as the CGLMP inequality given by $I_{\mathcal{B}_d}$. For the CGLMP it has been shown in [39] that it coincides with a family of equivalent facets. However, we do not know if the CGLMP inequality coincides with **all** facets of the polytope. Even though this might be the case, we cannot infer from this that all non-local states can be found with help of the CGLMP inequality because increasing the number of observables per party could define an improved polytope that could enable us to find even more non-local states. Please refer to [41] for a more detailed discussion.

Now let us investigate another property of the CGLMP inequality concerning the **maximal violation**. As we stated before, for the maximally entangled state $|\Omega_{0,0}\rangle$ the violation is maximal when the measurement setup is configured according to (2.49). However, in this case the largest eigenvalue of the corresponding Bell operator $\mathcal{B}_{I_d}$ is larger than the value $I_d\left(|\Omega_{0,0}\rangle\right)$ for all $d > 2$. The largest eigenvalues are summarised in this table (see [43]):

d	2	3	4	5	6	7
$I_d\left(|\Psi_{mv}\rangle\right)$	2.8284	2.9149	2.9727	3.0157	3.0497	3.0776
$I_d\left(|\Omega_{0,0}\rangle\right)$	2.8284	2.8729	2.8962	2.9105	2.9202	2.9272
difference [%]	0	1.4591	2.6398	3.6133	4.4345	5.1411

wherein $|\Psi_{mv}\rangle$ [7] denotes the eigenvector of $\mathcal{B}_{I_d}$ with the largest eigenvalue. Since all maximally entangled states are equivalent in terms of local unitaries (as discussed in §1.1.3) the state $|\Psi_{mv}\rangle$ must be non-maximally entangled[8]. For instance, for qutrits

---

[7] mv stands for "maximal violation"

[8] If $|\Omega_{0,0}\rangle = U_A \otimes U_B |\Psi_{mv}\rangle$ then we could use the Bell operator $U_A \otimes U_B \mathcal{B}_{I_d} U_A^\dagger \otimes U_B^\dagger$ to obtain $I_d\left(|\Omega_{0,0}\rangle\right) = I_d\left(|\Psi_{mv}\rangle\right)$ in contradiction to obtained values.

the eigenvector is the non-maximally entangled state $|\Psi_{mv}\rangle = \frac{1}{\sqrt{n}}\left(|00\rangle + \gamma |11\rangle + |22\rangle\right)$ with $n = 2 + \gamma^2$ and $\gamma = \left(\sqrt{11} - \sqrt{3}\right)/2$. Knowing that the states $|\Psi_{mv}\rangle$ yield stronger violations, we could ask if the above given values are the highest obtainable for I_d because the measurement configuration (2.49) has only been intended to be the best for $|\Omega_{0,0}\rangle$. Numerical investigations with varying states and measurement configurations show that these values are indeed the highest (see [43]). How can we interpret this result? Does the higher violation and the consequential higher resistance against noise signify that the states $|\Psi_{mv}\rangle$ are more non-local than $|\Omega_{0,0}\rangle$? This and further questions on the comparison of nonlocality and entanglement will be discussed in the next section.

2.4 Remarks on nonlocality and entanglement

A state ρ is said to be **non-local** if it violates a Bell inequality. Such a state is necessarily entangled, which follows from the fact that separable states cannot violate any Bell inequality. This can easily be seen by generalising the probability distribution (2.25). Recall that ideal Bell inequalities correspond to the facets of the polytope of local realistic correlations (2.77). The number of observables on each site depends on the regarded Bell inequality but we do not want to restrict ourself to the case of two observables. Thus, we generalise (2.25) to

$$P(A_1 = j, .., A_r = k, B_1 = l, .., B_s = m) , \qquad (2.78)$$

with $r, s \in \mathbb{N}$. According to (2.76), the normalisation defines a polytope and all local states belong to it. It is not difficult to recognise that any separable pure state belongs to the polytope: Since all probabilities are of product form $P(A_n = a, B_m = b) = P(A_n = a) \cdot P(B_m = b)$ (which is not the case when a state is entangled) we can easily construct the above stated probability distribution

$$P(A_1 = j, .., A_r = k, B_1 = l, .., B_s = m)$$
$$= P(A_1 = j) \cdots P(A_r = k) P(B_1 = l) \cdots P(B_s = m) , \qquad (2.79)$$

which of course obeys the normalisation relation due to normalised state vectors. Since separable mixed states are only convex combinations of pure ones we conclude that they belong to the polytope as well. This completes the proof that separable states cannot violate any Bell inequality. As a consequence, the operator $[2 \cdot \mathbb{1} - \mathcal{B}_{I_d}] \in \mathcal{H}_{HS}^{AB}$ is a entanglement witness because $Tr(\rho \mathcal{B}_{I_d}) \leq 2$ holds for all separable states. However, in general this is not an optimal witness, even if $\mathcal{B}_{I_d}$ is optimised for ρ.

Let us go back to the main subject of this section. Entanglement is a necessary component for nonlocality, however not all entangled states violate a Bell inequality. This will become more obvious when we discuss the geometry of entanglement and nonlocality in §3. At this point, we mention one famous example of an entangled state which does not violate the CHSH inequality: The Werner state $\rho_W = p|\Psi^-\rangle\langle\Psi^-| + \frac{1-p}{4}\mathbb{1}$ (for d=2 equivalent to the isotropic state) is entangled for $\frac{1}{3} < p \leq 1$, however violation of the CHSH inequality is obtained only for $\frac{1}{\sqrt{2}} < p \leq 1$[9]. This means that for $\frac{1}{3} < p \leq \frac{1}{\sqrt{2}}$ the statistical predictions can be reproduced by a local realistic theory, even though the state is entangled. This brings us to the notion of **hidden nonlocality**. We can claim that any distillable

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[9]The values of the parameter p can easily be verified with the PPT criterion and the Horodecki violation criterion

state (§1.4.3) contains some amount of nonlocality since we could perform local operations and classical communication (§1.4.2) until nonlocality is revealed. Despite this argument, the distinction between nonlocality and entanglement is not entirely clarified. Besides the fact that we do not know if any entangled state behaves non-locally in a particular measurement situation, there are some well-known examples that indicate that they might not be exactly the same. Eberhard has shown that non-maximally entangled states require lower detection efficiencies than maximally entangled ones, in order to close the detection loophole (see [42]). We have also seen that some non-maximally entangled states seem to be more non-local than the Bell states, due to their higher violation of the CGLMP inequality. With regard to this issue, one might argue that the resistance against noise is not a good measure of nonlocality. Some remarks on this can be found in a publication by Acin, Durt, Gisin and Latorre [43]. Nevertheless, they also suggest that a Bell inequality with more than two measurement instruments on each site could avoid this peculiarity. Another hint that entanglement and nonlocality are different resources has been found by Brunner, Gisin and Scarani (see [44]). They have shown that the simulation of non-maximally entangled states via **non-local machines** requires more resources than the simulation of a Bell state. The hypothetical non-local machine[10] was constructed to obtain the algebraic bound of the CHSH inequality without violating the non-signaling condition. Alice and Bob each have an input (x and y) and an output (a and b). Alice can choose the value of $x \in \{0,1\}$ and gets $a \in \{0,1\}$ in return, while Bob can choose the value of $y \in \{0,1\}$ and gets $b \in \{0,1\}$ in return.

Alice $x \in \{0,1\}$ →   non-local machine   ← $y \in \{0,1\}$ Bob

$a \in \{0,1\}$ ← $(a+b) \bmod 2 = x \cdot y$ → $b \in \{0,1\}$
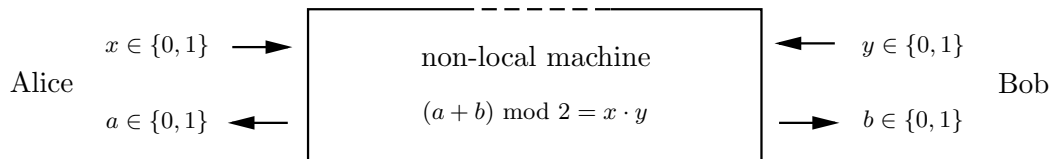
Figure 2.2: Schematic illustration of the non-local machine

The machine creates a random output $P(a=0) = P(a=1) = P(b=0) = P(b=1) = \frac{1}{2}$, though with a and b correlated according to the rule

$$(a+b) \bmod 2 = x \cdot y \ . \tag{2.80}$$

For instance, if $x = y = 0$ then the output of the machine is $a = b = 0$ in half the cases and $a = b = 1$ in the other half. Due to the local randomness this box cannot be used for signaling. Let us investigate the violation of the CHSH inequality. We assume that for any observable $A(\vec{a})$ there is a corresponding value for $x(\vec{a}) \in \{0,1\}$, and the same applies to $B(\vec{b})$ and $y(\vec{b}) \in \{0,1\}$. As before, we define a correlation function that yields the value 1 when the outputs a and b are identical, and -1 when they are different

$$C\left(A(\vec{a}), B(\vec{b})\right) \equiv \begin{cases} 1 & \text{for} \ \ a = b \\ -1 & \text{for} \ \ a \neq b \ . \end{cases} \tag{2.81}$$

For the case $A(\vec{a}) \to x(\vec{a}) = 1, A(\vec{a'}) \to x(\vec{a'}) = 0, B(\vec{b}) \to y(\vec{b}) = 0$ and $B(\vec{b'}) \to y(\vec{b'}) = 1$ the expectation values of the correlation function are $E(\vec{a}, \vec{b}) = E(\vec{a'}, \vec{b}) =$

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[10]other common names are PR box (named after Popescu and Rohrlich) and non-local box

$E(\vec{a'}, \vec{b'}) = 1$ and $E(\vec{a}, \vec{b'}) = -1$. Under such circumstances, the CHSH inequality yields the algebraic bound

$$|E(\vec{a}, \vec{b}) - E(\vec{a}, \vec{b'}) + E(\vec{a'}, \vec{b'}) + E(\vec{a'}, \vec{b})| = 4 \ . \tag{2.82}$$

This is the most non-local behaviour of a system possible. Thus, from a information-theoretical point of view, this machine can be seen as a resource of nonlocality. Inspired by this idea, Cerf, Gisin, Massar and Popescu have shown that quantum entanglement can be simulated without communication by use of the non-local machine (see [45]). Subsequent work demonstrated that for the simulation of a Bell state only one non-local machine is required, while at least two are required to simulate non-maximally entangled states (see [44]). This is another fact that strengthens the conjecture that there is a difference between nonlocality and entanglement. Further open questions concerning Bell inequalities, including also the experimental point of view, can be found in a publication by N. Gisin [46].

3 Geometrical aspects of bipartite systems

As the state space in quantum physics is a complex Hilbert-Schmidt space $\mathcal{H}_{HS}$ it is in general difficult to get a feeling for the properties of density matrices. However, in some cases they can be represented by vectors in a real vector space. For example, in §1.1 we have shown that density matrices can be described by real Bloch vectors. Due to the fact that the dimension of this vector is $d^2 - 1$, this representation is not very helpful if we intend to investigate bipartite systems. This is because even for the simplest case of two qubits the vector space is 15 dimensional. In this section we show that it is still possible to find attractive illustrations when it comes to studying entanglement and nonlocality of bipartite systems.

3.1 Geometry of the two-qubit system - the tetrahedron

3.1.1 Introduction

As usual, we begin with the bipartite qubit system (the following approach can be found in [47] and [48]). According to (1.16), any density matrix acting on $\mathcal{H}^{AB} = \mathbb{C}^2 \otimes \mathbb{C}^2$ can be written in the form

$$\rho = \frac{1}{4}(\mathbb{1} \otimes \mathbb{1} + \vec{r} \cdot \vec{\sigma} \otimes \mathbb{1} + \mathbb{1} \otimes \vec{s} \cdot \vec{\sigma} + \sum_{n,m=1}^{3} t_{nm}\sigma_n \otimes \sigma_m) \ . \tag{3.1}$$

Separability and nonlocality are invariant under local unitary transformations $U_A \otimes U_B$, therefore we can define equivalence classes of states

$$[\rho] = \{\rho'|\rho' = U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger\} \tag{3.2}$$

that have the same properties concerning separability and nonlocality. We exploit the group isomorphism between $SU(2)$ and $SO(3)$ which induces that for any $O \in SO(3)$ there exists a $U \in SU(2)$ that obeys

$$U\vec{n} \cdot \vec{\sigma} U^\dagger = (O\vec{n}) \cdot \vec{\sigma} \ . \tag{3.3}$$

Under a transformation $U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger$ the vectors $\vec{r}, \vec{s}$ and the matrix $T = (t_{nm})$ then become

$$\vec{r'} = O_A\vec{r} \ , \tag{3.4}$$

$$\vec{s'} = O_A\vec{s} \ , \tag{3.5}$$

$$T' = O_A T O_B^T \ . \tag{3.6}$$

According to the **singular value decomposition**, there exist orthogonal matrices O_A and O_B so that T' becomes diagonal with real entries. We choose density matrices ρ with diagonal $T = diag(t_{11}, t_{22}, t_{33})$ as the representatives of the equivalence classes $[\rho]$. Hence, for determining separability and nonlocality it suffices to investigate the set of states with diagonal T which we denote by $\mathcal{D}$. We write the diagonal entries in a vector $\vec{t} = (t_{11}, t_{22}, t_{33})$, in this way a density matrix $\rho \in \mathcal{D}$ is described by three vectors $\vec{r}, \vec{s}, \vec{t} \in \mathbb{R}^3$. Now, let us look through the elements of $\mathcal{D}$. Non-negativity is a necessary condition for a density matrix ρ, i.e. $Tr(|\Psi\rangle\langle\Psi|\rho) \geq 0$ for all $|\Psi\rangle \in \mathcal{H}^{AB}$. Consider the four projectors $P_1 = |\Psi^+\rangle\langle\Psi^+|$, $P_2 = |\Psi^-\rangle\langle\Psi^-|$, $P_3 = |\Phi^+\rangle\langle\Phi^+|$ and $P_4 = |\Phi^-\rangle\langle\Phi^-|$ given by the

Bell states $|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle)$ and $|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$. The Pauli matrix decomposition (1.23) yields $r_i = 0$ and $s_i = 0$ for $i \in \{1, 2, 3\}$ and

$$P_1 = |\Psi^+\rangle\langle\Psi^+| \qquad \Leftrightarrow \qquad \vec{t_1} = (+1, +1, -1) \, , \tag{3.7}$$

$$P_2 = |\Psi^-\rangle\langle\Psi^-| \qquad \Leftrightarrow \qquad \vec{t_2} = (-1, -1, -1) \, , \tag{3.8}$$

$$P_3 = |\Phi^+\rangle\langle\Phi^+| \qquad \Leftrightarrow \qquad \vec{t_3} = (+1, -1, +1) \, , \tag{3.9}$$

$$P_4 = |\Phi^-\rangle\langle\Phi^-| \qquad \Leftrightarrow \qquad \vec{t_4} = (-1, +1, +1) \, . \tag{3.10}$$

For two states ρ and ρ' given in the Pauli matrix decomposition we can compute $Tr(\rho\rho')$ easily, because it simplifies to $Tr(\rho\rho') = \frac{1}{4}(1 + \vec{r} \cdot \vec{r}' + \vec{s} \cdot \vec{s}' + Tr(TT'^\dagger))$. Thus, the four inequalities $Tr(P_n\rho) \geq 0$ with $n \in \{1, .., 4\}$ give

$$1 + t_{11} + t_{22} - t_{33} \geq 0 \, , \tag{3.11}$$

$$1 - t_{11} - t_{22} - t_{33} \geq 0 \, , \tag{3.12}$$

$$1 + t_{11} - t_{22} + t_{33} \geq 0 \, , \tag{3.13}$$

$$1 - t_{11} + t_{22} + t_{33} \geq 0 \, . \tag{3.14}$$

This restricts any $\vec{t}$ of $\rho \in \mathcal{D}$ to belong to a **regular tetrahedron** spanned by the Bell states at the vertices (see Fig.3.1). Note that only in the case where $\vec{r} = 0$ and $\vec{s} = 0$ the density matrices $\rho \in \mathcal{D}$ are diagonal in the Bell basis $\{|\Psi^+\rangle, |\Psi^-\rangle, |\Phi^+\rangle, |\Phi^-\rangle\}$ and only then the constraints (3.11)-(3.14) are also sufficient for non-negativity. States with this property define a subset LMM $\subset \mathcal{D}$ and are called **locally maximally mixed** because the respective reduced density matrices are maximally disordered $Tr_A(\rho) = Tr_B(\rho) = \frac{1}{2}\mathbb{1}$. The subset LMM $\subset \mathcal{D}$ contains only four pure states, namely the four Bell states, which can easily be seen by testing the purity condition

$$Tr(\rho^2) = \frac{1}{4}(1 + t_{11}^2 + t_{22}^2 + t_{33}^2) \overset{!}{=} 1 \tag{3.15}$$

$$\Rightarrow t_{11}^2 + t_{22}^2 + t_{33}^2 = 3 \, . \tag{3.16}$$

Geometrically spoken this defines a sphere with radius $\sqrt{3}$ that intersects the tetrahedron at the vertices, which therefore are the only pure sates of LMM.

$|\Phi^-\rangle\langle\Phi^-|$

$|\Phi^+\rangle\langle\Phi^+|$

$|\Psi^+\rangle\langle\Psi^+|$

$|\Psi^-\rangle\langle\Psi^-|$
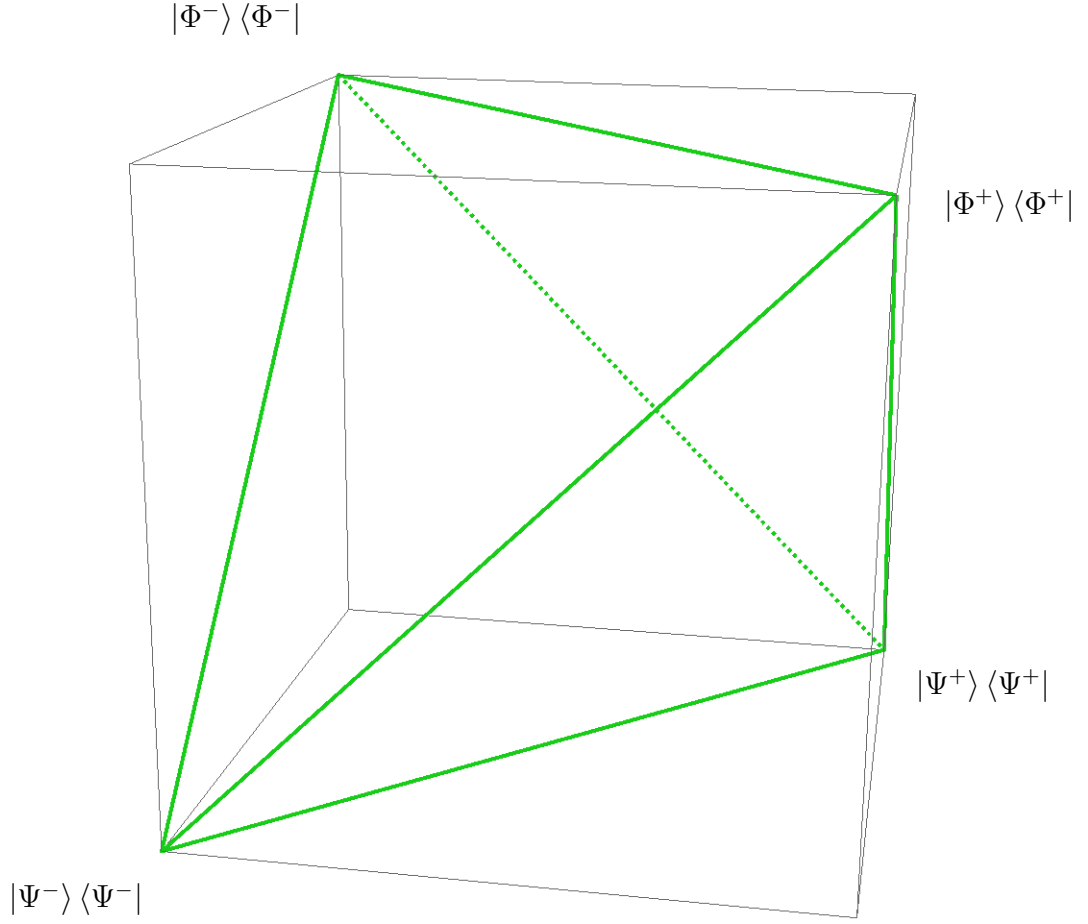
Figure 3.1: Illustration of the regular tetrahedron (green)

3.1.2 Geometry of separable and entangled states

Now, let us study the separability of $\rho \in$ LMM. In §1.2.2 we stated that the PPT criterion is a necessary and sufficient criterion for separability for density matrices acting on $\mathcal{H}^{AB} = \mathbb{C}^2 \otimes \mathbb{C}^2$. In the Pauli matrix decomposition it is trivial to compute the partial transposition. σ_1 is a symmetric matrix and therefore invariant under transposition, the same applies to σ_3 which is diagonal. Only σ_2 changes its algebraic sign $\sigma_2^T = -\sigma_2$, since it is anti-symmetric. Consequently, partial transposition results in a reflection of the tetrahedron where the coordinates are transformed according to $(t_{11}, t_{22}, t_{33}) \rightarrow (t_{11}, -t_{22}, t_{33})$. All operators $\rho \in$ LMM belonging to the original tetrahedron are non-negative, while the reflected tetrahedron contains operators ρ with negative eigenvalues. This means that all states ρ belonging to the cross section of the two tetrahedron are separable, while the other states are entangled. This intersection is an **octahedron** (see Fig.3.2). The extremal separable points have the coordinates $\vec{t}_{1/2} = (0, 0, \pm 1), \vec{t}_{3/4} = (0, \pm 1, 0)$ and $\vec{t}_{5/6} = (0, 0, \pm 1)$ and are 1:1 mixtures of two Bell states. A possible decomposition into a convex combination of separable density matrices can easily be found. Consider the mixture $\rho = \frac{1}{2}(\rho_1 + \rho_2)$ of the separable states $\rho_1 = \frac{1}{2}(\mathbb{1} + \vec{a} \cdot \vec{\sigma}) \otimes \frac{1}{2}(\mathbb{1} + \vec{b} \cdot \vec{\sigma})$ and $\rho_2 = \frac{1}{2}(\mathbb{1} - \vec{a} \cdot \vec{\sigma}) \otimes \frac{1}{2}(\mathbb{1} - \vec{b} \cdot \vec{\sigma})$.

A short computation gives

$$\rho = \frac{1}{2}(\rho_1 + \rho_2) = \frac{1}{4}(\mathbb{1} + \vec{a} \cdot \vec{\sigma} \otimes \vec{b} \cdot \vec{\sigma}) \ . \tag{3.17}$$

With the vectors $\vec{a} = \vec{e}_n$ and $\vec{b} = \pm \vec{e}_n$, where $\vec{e}_n$ stands for the unit vectors $\vec{e}_1 = (1,0,0)$, $\vec{e}_2 = (0,1,0)$ and $\vec{e}_3 = (0,0,1)$, we can explicitly demonstrate the separability of the extremal points of the octahedron, thus all states within the octahedron because they are just convex combinations of these points.
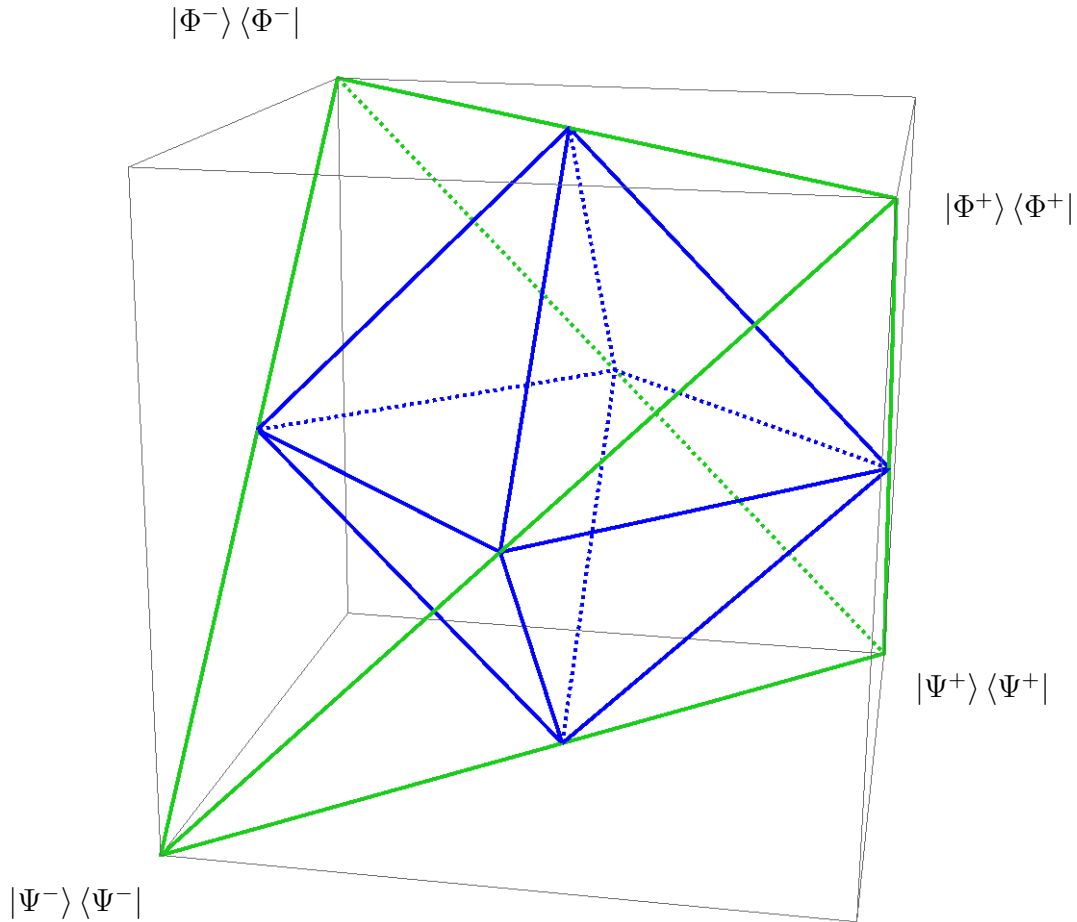
Figure 3.2: Illustration of the tetrahedron (green) and the octahedron of separable states (blue)

3.1.3 Geometry of non-local states

We intend to find the non-local states within the tetrahedron, i.e. states that violate the CHSH inequality[11]. For the bipartite qubit system this is not demanding because we can exploit the Horodecki violation criterion (2.24). First, we have to compute the eigenvalues of the matrix $K = T^T T$. Since T is already diagonal we get $\lambda_1 = t_{11}^2$, $\lambda_2 = t_{22}^2$ and $\lambda_3 = t_{33}^2$. A sufficient condition for nonlocality is that the sum of two eigenvalues is larger than 1 which implies the validity of at least one of the three

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[11]CHSH is equivalent to CGLMP for d=2

inequalities

$$t_{11}^2 + t_{22}^2 > 1 \ , \tag{3.18}$$

$$t_{11}^2 + t_{33}^2 > 1 \ , \tag{3.19}$$

$$t_{22}^2 + t_{33}^2 > 1 \ . \tag{3.20}$$

Each of the inequalities defines a cylinder with radius 1 in the geometric picture and a density matrix ρ that lies outside of one of them is non-local. The union of the exterior regions of these three cylinders is the set of non-local states (see Fig.3.3).
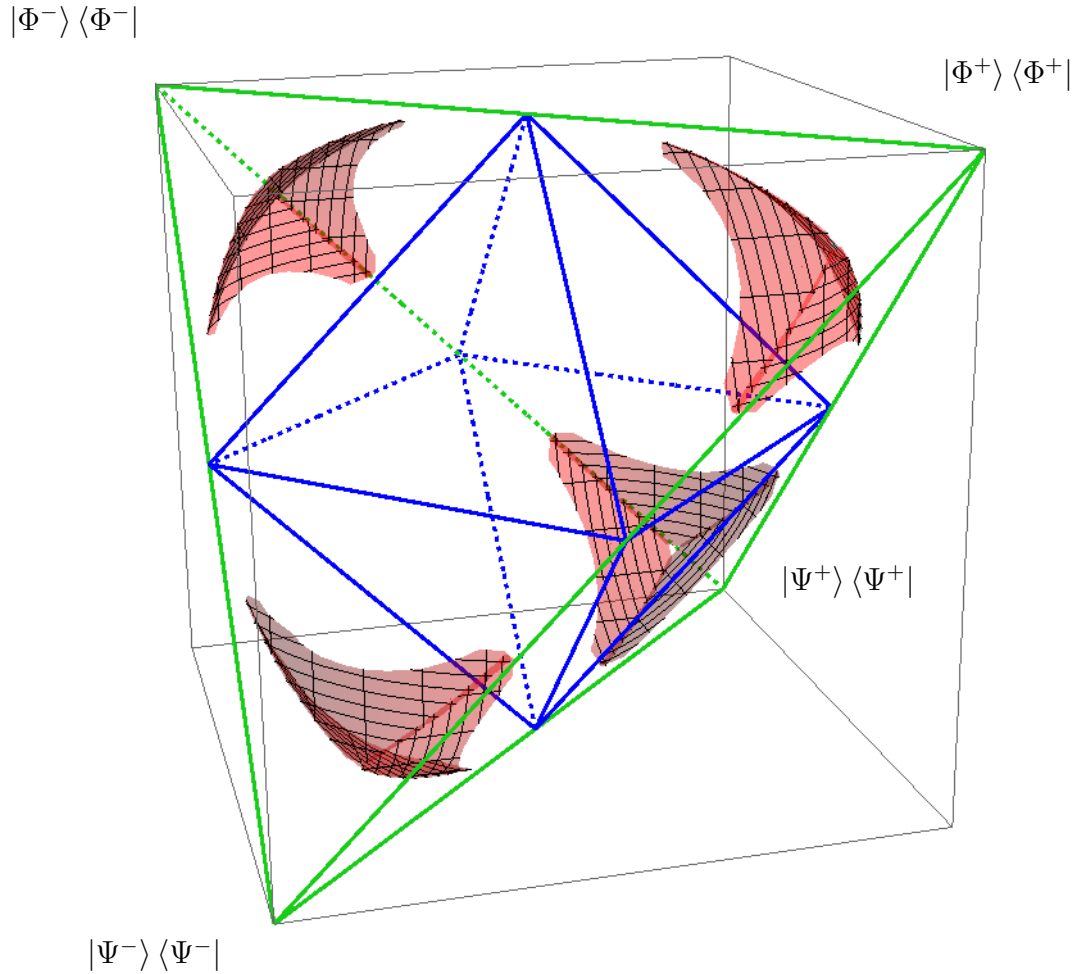
Figure 3.3: Illustration of the tetrahedron and the borders of nonlocality. States ρ beyond the red/meshed surfaces violate the CHSH inequality.

This descriptively illustrates that not all entangled states violate the CHSH inequality and that Bell operators $\mathcal{B}_{CHSH}$ are non-optimal entanglement witnesses for LMM states.

3.2 Geometry of bipartite qudit systems - the magic simplex

3.2.1 Introduction

The derivation of the octahedron was direct and straight forward. In seeking a similar geometric object for qudits we definitely try to proceed analogously. The first step is to express $\rho \in \mathcal{H}_{HS}^{AB}$ in the generalised form of (1.16) which is (1.43)

$$\rho = \frac{1}{d^2} \left(\mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{d^2-1} r_i \Gamma_i \otimes \mathbb{1} + \sum_{i=1}^{d^2-1} s_i \mathbb{1} \otimes \Gamma_i + \sum_{i,j=1}^{d^2-1} t_{ij} \Gamma_i \otimes \Gamma_j \right) . \qquad (3.21)$$

As we require a real vector space for a geometric structure, we use the generalised Gell-Mann matrices for $\{\Gamma_i\}$. In order to use the same notation as for qubits, we express ρ with generalised Bloch vectors $\vec{r}_\Lambda$, $\vec{s}_\Lambda$ and a correlation matrix $T = (t_{ij})$

$$\rho = \frac{1}{d^2} \left(\mathbb{1} \otimes \mathbb{1} + \vec{r}_\Lambda \cdot \vec{\Lambda} \otimes \mathbb{1} + \mathbb{1} \otimes \vec{s}_\Lambda \cdot \vec{\Lambda} + \sum_{i,j=1}^{d^2-1} t_{ij} \Gamma_i \otimes \Gamma_j \right) . \qquad (3.22)$$

The next step would be the diagonalisation of the matrix $T = (t_{ij})$ via two orthogonal matrices O_A and O_B. However, here we are confronted with the problem that the relation $U \vec{r}_\Lambda \cdot \vec{\Lambda} U^\dagger = (O \vec{r}_\Lambda) \cdot \vec{\Lambda}$ is invalid for Gell-Mann matrices. For example, consider the state $\rho = \frac{1}{3}(\mathbb{1} + \vec{b}_\Lambda \cdot \vec{\Lambda})$ with $\vec{b}_\Lambda^T = (0,0,1,0,0,0,0,0)$

$$\rho = \frac{1}{3}(\mathbb{1} + \lambda_3) = \begin{pmatrix} \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} \end{pmatrix} , \qquad (3.23)$$

which is obviously a valid density matrix. Let us assume that there exists a unitary transformation $\rho' = U \rho U^\dagger = \frac{1}{3}(\mathbb{1} + U \vec{b}_\Lambda \cdot \vec{\Lambda} U^\dagger) = \frac{1}{3}(\mathbb{1} + (O\vec{r}_\Lambda) \cdot \vec{\Lambda})$ that corresponds to the orthogonal matrix O

$$O = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \Rightarrow \qquad \vec{b}'_\Lambda = O\vec{r}_\Lambda = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} . \qquad (3.24)$$

This transformation turns the state ρ into $\rho' = \frac{1}{3}(\mathbb{1} + \vec{b}'_\Lambda \cdot \vec{\Lambda})$

$$\rho' = \frac{1}{3}(\mathbb{1} + \lambda_8) = \begin{pmatrix} \frac{1}{3}\left(1 + \frac{1}{\sqrt{3}}\right) & 0 & 0 \\ 0 & \frac{1}{3}\left(1 + \frac{1}{\sqrt{3}}\right) & 0 \\ 0 & 0 & \frac{1}{3}\left(1 - \frac{2}{\sqrt{3}}\right) \end{pmatrix} . \qquad (3.25)$$

As we can see the eigenvalues of ρ and ρ' are not the same, which in other words means that the orthogonal transformation O results in a non-unitary transformation[12] of ρ. Hence, the relation $U \vec{r}_\Lambda \cdot \vec{\Lambda} U^\dagger = (O \vec{r}_\Lambda) \cdot \vec{\Lambda}$ cannot be valid. Even if

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[12]Eigenvalues are invariant under unitary transformations

T can be diagonalised by product unitary transformations $U_A \otimes U_B$ for a subset of LMM states there is another problem. Consider a locally maximally mixed state $\rho \in$ LMM [13] with diagonal T

$$\rho = \frac{1}{d^2} \left(\mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{d^2-1} t_{ii} \Gamma_i \otimes \Gamma_j \right) . \qquad (3.26)$$

In the qubit case the eigenvectors of ρ are the Bell states for an arbitrary choice of $\{t_{ii}\}$, thus the non-negativity condition leads to a simple geometric figure, namely the tetrahedron. For qudits the situation is different because the eigenvectors of ρ depend on $\{t_{ii}\}$ implying that the geometric figure given by non-negativity is much more difficult to determine. Due to this and the fact that the set of states whose correlation matrices T can be diagonalised via local unitaries are merely a subset of LMM, we choose another subset of LMM whose properties concerning entanglement are interesting and whose non-negativity is easier to handle.

At this point we adopt the way of B. Baumgartner, B.C. Hiesmayr and H. Narnhofer, who introduced a generalisation of the tetrahedron for qudits [49]. As the octahedron is spanned by the four Bell states, the expansion for higher dimensional systems is the so called **magic simplex** spanned by generalised Bell states $P_{k,l} = |\Omega_{k,l}\rangle \langle \Omega_{k,l}|$ with $|\Omega_{k,l}\rangle = (W_{k,l} \otimes \mathbb{1}) |\Omega_{0,0}\rangle$ given by the Weyl operators (1.31)

$$\mathcal{W} = \{ \sum_{k,l=0}^{d-1} c_{k,l} P_{k,l} \mid c_{k,l} \geq 0, \sum_{k,l=0}^{d-1} c_{k,l} = 1 \} . \qquad (3.27)$$

This simplex is a convex set located in a $d^2 - 1$ dimensional hyperplane in a d^2 dimensional real vector space of hermitian operators spanned by the operators $\{P_{k,l}\}$. When the element $\rho \in \mathcal{W} \subset \mathcal{H}_{HS}^{AB}$ is expressed in the basis $\{|\Omega_{k,l}\rangle\} \in \mathcal{H}^{AB}$ it becomes obvious that the only pure states in $\mathcal{W}$ lie at the vertices $\{P_{k,l}\}$ (diagonal ρ). Before we investigate the states within the magic simplex let us specify the subset of LMM states belonging to it. One requirement for the existence of a representative in $\mathcal{W}$ surely is that $\rho \in$ LMM must be decomposable into orthogonal Bell states. However, we now show why this is only a necessary and not a sufficient condition. Consider the unitary transformation $U = U_A \otimes U_B = \sum_s |s'\rangle \langle s| \otimes \mathbb{1}$ transforming a Bell state $|\Omega_{0,0}\rangle = \frac{1}{\sqrt{d}} \sum_s |s\rangle \otimes |s\rangle$ into another orthonormal Bell state $|\Phi\rangle = \frac{1}{\sqrt{d}} \sum_s |s'\rangle \otimes |s\rangle$. Orthogonality implies $Tr U_A = 0$ meaning the sum of all eigenvalues U_A has to be zero. Without loss of generality, we can set one of the eigenvalues 1 because we are free in choosing a global phase. This implies the rest of the eigenvalues for qubits and qutrits, while for $d \geq 4$ there are various ways for complying $Tr U_A = 0$. The Weyl operators $W_{k,l}$ have the eigenvalues $e^{i2\pi b/d}$ with $b \in \{0, .., d-1\}$ and if a state is decomposable into certain Bell states their intertwiners must have the same eigenvalues in order to have a representative in $\mathcal{W}$.

3.2.2 Symmetries and equivalences inside $\mathcal{W}$

We focus on local (anti-)unitary transformations $U_A \otimes U_B$ mapping $\mathcal{W}$ onto itself. In particular we are interested in equivalence classes $[\rho] = \{\rho' \in \mathcal{W} | \rho' = U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger\}$ of states within the magic simplex having the same properties concerning separability and nonlocality. These equivalences can best be studied

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[13]$LMM = \{\rho \in \mathcal{H}_{HS}^{AB} | \rho_A = Tr_B \rho = \rho_B = Tr_A \rho = \frac{1}{d} \mathbb{1} \}$

when the group structure of the Weyl operators and the concept of a finite discrete classical phase space are used. The Weyl operators originate from the quantization of classical kinematics where they are used for translations between discrete states in a phase space. Each point within this phase space corresponds to an index pair (k, l), where $l \in \{0, .., d-1\}$ denotes the quantum number of the position and $k \in \{0, .., d-1\}$ the quantum number of the momentum.
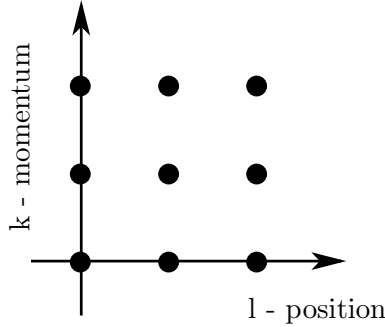

Figure 3.4: Illustration of the finite discrete classical phase space for $d = 3$.

Due to the fact that the Weyl operators have been used as the intertwiners between the vertices $\{P_{k,l}\}$ of the simplex we can exploit this phase space structure for our investigations, i.e. to each point (k, l) of the lattice in the phase space we assign a Bell state $P_{k,l}$. We know by construction that any Bell state $P_{k,l}$ can be mapped onto any $P_{k',l'}$ by use of a certain Weyl operator $U = W_{m,n} \otimes \mathbb{1}$ with $k' = (k + m) \bmod d$ and $l' = (l + n) \bmod d$, meaning there are no restrictions on translations $\mathcal{T}$ in the phase space

$$ \mathcal{T} : \begin{pmatrix} k \\ l \end{pmatrix} \longrightarrow \begin{pmatrix} k' \\ l' \end{pmatrix} . \tag{3.28} $$

There are even more local unitary transformations mapping $\mathcal{W}$ onto itself such as $U_\mathcal{R} \otimes U_\mathcal{R}^*$ with

$$ U_\mathcal{R} = \frac{1}{d} \sum_{s,t=0}^{d-1} w^{-st} |t\rangle \langle s| . \tag{3.29} $$

Under this transformation the Bell states $P_{k,l}$ become

$$ U_\mathcal{R} \otimes U_\mathcal{R}^* P_{k,l} U_\mathcal{R}^\dagger \otimes U_\mathcal{R}^T = P_{l,k} . \tag{3.30} $$

Thus, this is a **quarter rotation** around the origin in the phase space picture

$$ \mathcal{R} : \begin{pmatrix} k \\ l \end{pmatrix} \longrightarrow \begin{pmatrix} l \\ k \end{pmatrix} . \tag{3.31} $$

The next transformation we consider is $U_\mathcal{V} \otimes U_\mathcal{V}^*$ with

$$ U_\mathcal{V} = \sum_{s=0}^{d-1} w^{-s(s+d)/2} |s\rangle \langle s| . \tag{3.32} $$

This affects the Bell states in the following way

$$ U_\mathcal{V} \otimes U_\mathcal{V}^* P_{k,l} U_\mathcal{V}^\dagger \otimes U_\mathcal{V}^T = P_{k+l,l} . \tag{3.33} $$

In the phase space this is a **vertical shear**

$$\mathcal{V} : \begin{pmatrix} k \\ l \end{pmatrix} \longrightarrow \begin{pmatrix} k+l \\ l \end{pmatrix} . \tag{3.34}$$

Another realisable mapping is the **vertical reflection** $\mathcal{S}$

$$\mathcal{S} : \begin{pmatrix} k \\ l \end{pmatrix} \longrightarrow \begin{pmatrix} -k \\ l \end{pmatrix} . \tag{3.35}$$

The corresponding anti-unitary transformation on the Hilbert space $\mathcal{H}^{AB}$ is the tensorial product of local complex conjugation C

$$\sum_{s=0}^{d-1} a_s \, |s\rangle \longrightarrow \sum_{s=0}^{d-1} a_s^* \, |s\rangle . \tag{3.36}$$

The composite application $C \otimes C$ of this anti-unitary transformation onto the $P_{k,l}$ yields the desired vertical reflection

$$C \otimes C P_{k,l} C^\dagger \otimes C^\dagger = P_{-k,l} . \tag{3.37}$$

The three transformations $\mathcal{R}, \mathcal{V}, \mathcal{S}$ together with the translation $\mathcal{T}$ are the generating elements of an arbitrary phase space transformation of form (see [49])

$$\begin{pmatrix} k \\ l \end{pmatrix} \longrightarrow \begin{pmatrix} m & n \\ p & q \end{pmatrix} \begin{pmatrix} k \\ l \end{pmatrix} + \begin{pmatrix} j \\ r \end{pmatrix} \qquad M = \begin{pmatrix} m & n \\ p & q \end{pmatrix} , \tag{3.38}$$

with $det(M) = 1$ or $det(M) = d - 1$. For $det(M) = 1$ the corresponding transformation acting on the Hilbert space $\mathcal{H}^{AB}$ is unitary, for $det(M) = d - 1$ it is anti-unitary. Hence, further transformations as for instance horizontal shear, squeezing, horizontal or diagonal reflection with varying origins can be decomposed into $\mathcal{T}, \mathcal{R}, \mathcal{V}$ and $\mathcal{S}$ and a representation acting on $\mathcal{H}^{AB}$ can be constructed out of them. Transformations that cannot be written in the form (3.38) or that do not obey $det(M) = 1$ (or $d - 1$) are excluded because they do not possess local (anti-)unitary representations. A detailed proof of this fact from a group theoretical point of view can be found in [49].
Let us briefly point out some major consequences of these equivalences. In most cases we study low dimensional sections of the simplex. These slices are mainly mixtures of particular $P_{k,l}$'s and the unity $\mathbb{1}$ which is an equally weighted mixture of all Bell states $\mathbb{1} = \sum_{k,l=0}^{d-1} P_{k,l}$ and can be regarded as uncolored noise. The transformation rules imply that all one parameter states $\rho = \frac{1-\alpha}{d^2}\mathbb{1} + \alpha P_{k,l}$ with arbitrary $k, l \in \{0, .., d - 1\}$ but same α have the properties in terms of separability and (non-)locality (Identity $\mathbb{1}$ is mapped onto itself for all unitary transformations and the single Bell state $P_{k,l}$ can be translated freely). These are the so-called **isotropic states**. The same applies to two-parameter families of states of form $\rho = \frac{1-\alpha-\beta}{d^2}\mathbb{1} + \alpha P_{k,l} + \beta P_{m,n}$ with arbitrary $k, l, m, n \in \{0, .., d - 1\}$. We translate the first point (k, l) to the origin $(0, 0)$ and then bring the second point $(m - k, n - l)$ to $(0, 1)$. This can be done by the matrix $M = \begin{pmatrix} n - l & k - m \\ 0 & q \end{pmatrix}$ with $q(n - l) = 1 = det(M)$. As a result we have found that such states with different $P_{k,l}$ and $P_{m,n}$ but same α and β are equivalent and furthermore they are symmetric in α and β (i.e. apply the same procedure but interchange the roles of the points). For

three-parameter states $\rho = \frac{1-\alpha-\beta-\gamma}{d^2}\mathbb{1} + \alpha P_{k,l} + \beta P_{m,n} + \gamma P_{p,q}$ the situation changes. We can proceed as before bringing two points to $(0,0)$ and $(0,1)$. If the third point was on a line $\{(k,l),(m,n),(p,q) = (a(m-k)+k, a(n-l)+l)\}$ then it is now on the line with $k = 0$ due to linearity of M, for instance for d=3 this point takes on $(0,2)$. If it was not an element of this line it can be brought to $(1,0)$ with horizontal shear and vertical reflection without influencing the points on $k = 0$. However, it cannot be brought to $k = 0$ without transforming the other two points. This shows that not all three parameter states with same α, β and γ necessarily possess the same attributes. We do not discuss cases with more than three points in detail but want to stress that all complete lines $\{(k,l),(m,n),..,((d-1)\cdot(m-k)+k,(d-1)\cdot(n-l)+l)\}$ are equivalent because they can all be mapped onto the line $\{(0,0),(0,1),..,(0,d-1)\}$ by transforming two of the points onto $(0,0)$ and $(0,1)$ with the above stated method.
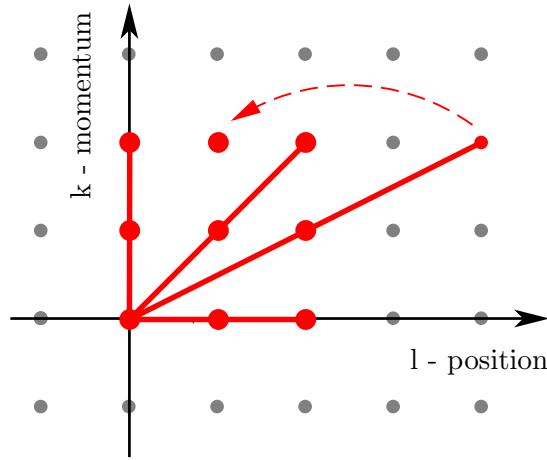
Figure 3.5: Illustration of all possible complete lines through the point $(0,0)$ for $d = 3$. Lines can be completed by points with $k,l \notin \{0,..,d-1\}$ because of the periodicity of the Weyl operators implying $P_{k,l} = P_{k+m\cdot d,l+n\cdot d}$ for all $n,m \in \mathbb{Z}$

3.2.3 Geometry of separable and entangled states

Theoretical strategies for determining the separable and entangled states within $\mathcal{W}$ are discussed and applied onto sections of the simplex for $d = 3$. We begin with entangled states ρ that can be revealed by the PPT criterion (see §1.2.2) and provide some simplifications for determining definiteness of operators ρ^{T_A} that are inferred from the structure of the simplex $\mathcal{W}$. The explicit form of a projector $P_{k,l}$ is

$$P_{k,l} = \frac{1}{d}\sum_{s,t=0}^{d-1} w^{k(s-t)}\,|s-l,s\rangle\,\langle t-l,t|\ . \tag{3.39}$$

Therefore the elements of $\mathcal{W}$ are

$$\rho = \frac{1}{d}\sum_{s,t,k,l=0}^{d-1} c_{k,l}w^{k(s-t)}\,|s-l,s\rangle\,\langle t-l,t| \tag{3.40}$$

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and partial transposition on subsystem A gives

$$\rho^{T_A} = \frac{1}{d} \sum_{s,t,k,l=0}^{d-1} c_{k,l} w^{k(s-t)} |t-l, s\rangle \langle s-l, t| \ . \tag{3.41}$$

We substitute the running index l by $l = s + t - m$ which leads to the expression

$$\begin{aligned}
\rho^{T_A} &= \frac{1}{d} \sum_{s,t,k,m=0}^{d-1} c_{k,s+t-m} w^{k(s-t)} |m-s, s\rangle \langle m-t, t| \\
&= \sum_{m=0}^{d-1} \left[\frac{1}{d} \sum_{s,t,k=0}^{d-1} c_{k,s+t-m} w^{k(s-t)} |m-s, s\rangle \langle m-t, t| \right] \\
&= \sum_{m=0}^{d-1} B_m \ . \tag{3.42}
\end{aligned}$$

As we observe, each operator B_m acts on a subspace $\mathcal{H}_m = \mathbb{C}^d$ spanned by the vectors $\{|m-s\rangle \otimes |s\rangle\}_{s=0,..,d-1}$. Thus, for determining definiteness of ρ^{T_A} it suffices to consider the definiteness of the $d \times d$ matrices B_m having the entries

$$(B_m)_{s,t} = \frac{1}{d} \sum_{k=0}^{d-1} c_{k,s+t-m} w^{k(s-t)} \ . \tag{3.43}$$

Relations between the matrices B_m lead to further simplifications of this problem. For example

$$(B_{m-2})_{s,t} = \frac{1}{d} \sum_{k=0}^{d-1} c_{k,s+t-m+2} w^{k(s-t)} = (B_m)_{s+1,t+1} \tag{3.44}$$

holds for even and odd d and signifies that B_{m-2} and B_m are unitarily equivalent. Moreover, for odd d all B_m are unitarily equivalent which can be proven by using the periodicity (modulo d)

$$\begin{aligned}
(B_{m-1})_{s,t} &= \frac{1}{d} \sum_{k=0}^{d-1} c_{k,s+t-m+1} w^{k(s-t)} \\
&= \frac{1}{d} \sum_{k=0}^{d-1} c_{k,s+t-m+1+d} w^{k(s+(d+1)/2-t-(d+1)/2)} \\
&= (B_m)_{s+(d+1)/2,t+(d+1)/2} \ . \tag{3.45}
\end{aligned}$$

Since unitarily equivalent matrices have the same eigenvalues it suffices to compute the eigenvalues of a single B_m when the dimension d is odd and two B_m (one with odd m and one with even m) when the dimension d is even.

As we already know, we can exclude states ρ with non-positive ρ^{T_A} from being separable but positivity $\rho^{T_A} \geq 0$ does not guarantee their separability. We now show which states $\rho \in \mathcal{W}$ are separable with certainty. Consider functions $k_n(x)$ and $l_n(x)$ with $x \in \{0, .., d-1\}$ defining complete lines $\{(k_n(0), l_n(0)), .., (k_n(d-1), l_n(d-1))\}$. We state that all states that are equally weighted mixtures of states forming a

complete line are separable (in particular these are the outermost separable states of $\mathcal{W}$ as is shown in [50]).

$$\lambda_n = \frac{1}{d} \sum_{x=0}^{d-1} P_{k_n(x),l_n(x)} \quad \in \text{SEP} . \tag{3.46}$$

We have to prove this for one particular complete line only, for instance $k(x) = x$ and $l = 0$ because of their equivalence in terms of local unitaries (§3.2.2)

$$\lambda = \frac{1}{d} \sum_{x=0}^{d-1} P_{k=x,0}$$

$$= \frac{1}{d^2} \sum_{x,s,t=0}^{d-1} w^{x(s-t)} |s,s\rangle \langle t,t| . \tag{3.47}$$

Once again we use $\frac{1}{d} \sum_{x=0}^{d-1} w^{x(s-t)} = \delta_{s,t}$ and get

$$\rho_{line} = \frac{1}{d} \sum_{s=0}^{d-1} |s,s\rangle \langle s,s| , \tag{3.48}$$

which is obviously separable. All possible convex combinations of all line states λ_n (3.46) form the **kernel polytope (KP)**

$$\text{KP} = \left\{ \rho \in \mathcal{W} \mid \rho = \sum_n c_n \lambda_n , \ c_n \geq 0 , \ \sum_n c_n = 1 \right\} , \tag{3.49}$$

a subset of separable states of PPT$\cap\mathcal{W}$[14].

At this point the separability of states within the kernel polytope and the non-separability of NPPT states are ensured. For the remaining states that are PPT but do not lie within the kernel polytope we have to construct optimal entanglement witnesses $W_{opt.}$ if we want to completely clarify the question of separability. As we already know for all states ρ that lie on the boundary of the convex set of separable states ∂SEP there exists an optimal entanglement witness with $Tr(W_{opt.}\rho) = 0$ (§1.2.4). To determine the boundary states of SEP$\cap\mathcal{W}$ and their witnesses the symmetry of the simplex is of great help. Consider a state ρ which is invariant under the symmetry group $\mathcal{G}$ of unitary or anti-unitary operators $V_g \in \mathcal{G}$, meaning $V_g \rho V_g^{-1} = \rho$ for all g. Thus,

$$Tr(W\rho) = Tr(WV_g^{-1}V_g\rho V_g^{-1}V_g) = Tr(V_gWV_g^{-1}V_g\rho V_g^{-1}) = Tr(V_gWV_g^{-1}\rho)$$

shows that the symmetries $\mathcal{G}$ of a state ρ are reflected in its witnesses. In other words we can restrict the search for witnesses on $\mathcal{G}$-invariant operators $V_gWV_g^{-1} = W$ (for all g). This is a significant restriction on the form of the witness when the regarded state ρ is of high symmetry. In our case where all states belong to the magic simplex $\mathcal{W}$ all states are invariant under the symmetry group $\mathcal{G} = \{2P_{k,l} - \mathbb{1}\}_{k,l=0,..,d-1}$ and the most general form of an $\mathcal{G}$-invariant W is

$$W = \sum_{k,l} \kappa_{k,l} P_{k,l} \qquad \kappa_{k,l} \in \mathbb{R} . \tag{3.50}$$

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[14]When we speak of PPT as a set we mean PPT=$\{\rho \in \mathcal{H}_{HS}^{AB} \mid Tr(\rho) = 1, \rho \geq 0, \rho^{T_A} \geq 0 \}$

According to (1.64) W must have non-negative expectation values for all product states

$$\langle\psi|\otimes\langle\eta|\,W\,|\psi\rangle\otimes|\eta\rangle$$

$$=\frac{1}{d}\sum_{k,l,s,t=0}^{d-1}\kappa_{k,l}\,\langle\psi|\otimes\langle\eta|\,W_{k,l}\otimes\mathbb{1}\,|s\rangle\otimes|s\rangle\,\langle t|\otimes\langle t|\,W_{k,l}^{\dagger}\otimes\mathbb{1}\,|\psi\rangle\otimes|\eta\rangle$$

$$=\frac{1}{d}\sum_{k,l,s,t=0}^{d-1}\kappa_{k,l}\,\langle\psi|\,W_{k,l}\,|s\rangle\,\langle\eta|s\rangle\,\langle t|\eta\rangle\,\langle t|\,W_{k,l}^{\dagger}\,|\psi\rangle$$

$$=\frac{1}{d}\,\langle\psi|\left[\sum_{k,l=0}^{d-1}\kappa_{k,l}W_{k,l}\,|\phi\rangle\,\langle\phi|\,W_{k,l}^{\dagger}\right]|\psi\rangle$$

$$=\frac{1}{d}\,\langle\psi|\,M_{\phi}\,|\psi\rangle\geq 0 \qquad\qquad \forall\,|\psi\rangle\,,|\phi\rangle\in\mathbb{C}^{d}\ . \tag{3.51}$$

Here we have introduced a matrix M_{ϕ} that depends on the vector $|\phi\rangle=\sum_{s=0}^{d-1}\langle\eta|s\rangle\,|s\rangle$ which is merely an anti-unitary transformation of $|\eta\rangle$ (complex conjugation of the expansion coefficients of $|\eta\rangle$ in the basis $\{|s\rangle\}$). Consequently, if non-negativity of W holds for all $|\phi\rangle$ then it also holds for all $|\psi\rangle$ and vice versa. Iff W is not only an entanglement witness but also optimal, then there exists a product state $|\psi'\rangle\otimes|\eta'\rangle\in\mathcal{H}^{AB}$ so that

$$\langle\psi'|\otimes\langle\eta'|\,W\,|\psi'\rangle\otimes|\eta'\rangle=\frac{1}{d}\,\langle\psi'|\,M_{\phi'}\,|\psi'\rangle=0\ . \tag{3.52}$$

Since M_{ϕ} is non-negative the eigenvalue for $|\psi'\rangle$ must be zero and if this is the case then W is an optimal entanglement witness for $\rho=|\psi',\eta'\rangle\,\langle\psi',\eta'|$ and all incoherent superpositions that are compatible with the symmetry of W

$$\rho_{\mathcal{G}}=\sum_{g}c_{g}V_{g}\,|\psi',\eta'\rangle\,\langle\psi',\eta'|\,V_{g}^{-1} \qquad\qquad c_{g}\geq 0\ ,\ \sum_{g}c_{g}=1\ . \tag{3.53}$$

It follows that the boundary of SEP$\cap\mathcal{W}$ is determined by the innermost states of the set $\mathcal{W}$ obeying $Tr(W\rho)=0$, where W is an operator $W=\sum_{k,l}\kappa_{k,l}P_{k,l}$ whose associated non-negative matrices M_{ϕ} have at least one vanishing eigenvalue, i.e. $det(M_{\phi})=0$. Finding those innermost states is still a very difficult task even though symmetries have narrowed down the search for their optimal witnesses and in many cases one must perform a numerical variation of the parameters $\{\kappa_{k,l}\}$ and the vector $|\phi\rangle$. Analytical solutions can be obtained for states ρ with further symmetries. For instance, if we intend to find the boundary of the one-parameter family of states

$$\rho=\frac{1-\alpha}{d^{2}}\mathbb{1}+\alpha P_{0,0}\ , \tag{3.54}$$

which is invariant under all phase space transformations except translations, we can restrict the search for an optimal witness on $W=a\mathbb{1}+bP_{0,0}$ having the same symmetries. For this witness the associated matrix M_{ϕ} is

$$M_{\phi}=da\mathbb{1}+b\,|\phi\rangle\,\langle\phi|\ . \tag{3.55}$$

Here the eigenvalues do not depend on $|\phi\rangle$ and are $da+b$, da and da so one must choose $a>0$ and $b=-da$ in order to get an optimal W ($det(M_{\phi})=0$). The state

on the boundary of SEP is then given by

$$Tr(W\rho) = aTr\left[(\mathbb{1} - dP_{0,0})(\frac{1-\alpha}{d^2}\mathbb{1} + \alpha P_{0,0})\right]$$

$$= a\left[\frac{d-1-\alpha(d^2-1)}{d}\right] \stackrel{!}{=} 0 , \tag{3.56}$$

which is achieved for $\alpha = \frac{1}{d+1}$. It follows that all isotropic states $\rho = \frac{1-\alpha}{d^2}\mathbb{1} + \alpha P_{p,q}$ have this bound for α due to their equivalence by local unitaries (see §3.2.2). Their optimal entanglement witnesses $W = a\mathbb{1} - daP_{p,q}$ with $a > 0$ define the enclosure polytope. For an arbitrary state $\rho \in \mathcal{W}$ we compute

$$Tr(W\rho) = aTr\left[(\mathbb{1} - dP_{p,q})(\sum_{k,l=0}^{d-1} c_{k,l}P_{k,l})\right]$$

$$= a(-dc_{p,q} + \sum_{k,l}^{d-1} c_{k,l})$$

$$= a(-dc_{p,q} + 1) . \tag{3.57}$$

This implies that any ρ that has at least one component $c_{k,l} > \frac{1}{d}$ is detected to be entangled by one of the isotropic witnesses $W = a\mathbb{1} - daP_{p,q}$. Consequently, separable states lie within the so-called **enclosure polytope (EP)** defined by

$$\text{EP} = \left\{\rho \in \mathcal{W} \mid \frac{1}{d} \geq c_{k,l} \geq 0 \ \ \forall c_{k,l}\right\} . \tag{3.58}$$

We now study two and three dimensional sections of the simplex for $d = 3$ (qutrits) in order to illustrate regions of separable and entangled states that result from these concepts. The first family of states we consider is a mixture of two Bell states which are all locally unitarily equivalent to $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$. This means we have $c_{0,0} = \frac{1-\alpha-\beta}{9} + \alpha$, $c_{1,0} = \frac{1-\alpha-\beta}{9} + \beta$ and all other components are $c_{k,l} = \frac{1-\alpha-\beta}{9}$ which implies $\alpha \geq \frac{\beta-1}{8}$, $\beta \geq \frac{\alpha-1}{8}$ and $\beta \leq 1-\alpha$ for positivity of ρ. We obtain the boundary of PPT by setting $det(B_0) = 0$ which yields $(2\alpha + 2\beta + 1)(8\alpha^2 + 8\beta^2 - 11\beta\alpha + 2\alpha + 2\beta - 1) = 0$ (details on this and other computations regarding ρ can be found in the Appendix D). Due to invariance of ρ under horizontal reflection we restrict on entanglement witnesses of form $W = \lambda\frac{1}{3}\mathbb{1} + aP_{0,0} + bP_{1,0} + cP_{2,0}$. As it has been shown in this section, line states for example $\rho_{line} = \frac{1}{3}(P_{0,1} + P_{1,1} + P_{2,1})$ are separable. Hence, $Tr(W\rho_{line}) = \frac{\lambda}{3} \geq 0$ must always be valid and therefore λ cannot be negative. When we set $\lambda = 1$ (which only fixes the scaling of the witness) the associated matrix M_ϕ becomes $M_\phi = \mathbb{1} + aW_{0,0}|\phi\rangle\langle\phi|W_{0,0}^\dagger + bW_{1,0}|\phi\rangle\langle\phi|W_{1,0}^\dagger + cW_{2,0}|\phi\rangle\langle\phi|W_{2,0}^\dagger$. A numerical search for solutions of $det(M_\phi) = 0$ by varying the parameters a, b, c and the vector $|\phi\rangle$ was done in [51]. It is shown in [52] that there exist optimal witnesses $W_{opt.}$ so that $Tr(W_{opt.}\rho) = 0$ yields the boundaries $4\alpha^2 - 5\alpha + 40\beta^2 + (17\alpha - 14)\beta + 1 = 0$ and $4\beta^2 - 5\beta + 40\alpha^2 + (17\beta - 14)\alpha + 1 = 0$. Graphically this is illustrated in the following figures.
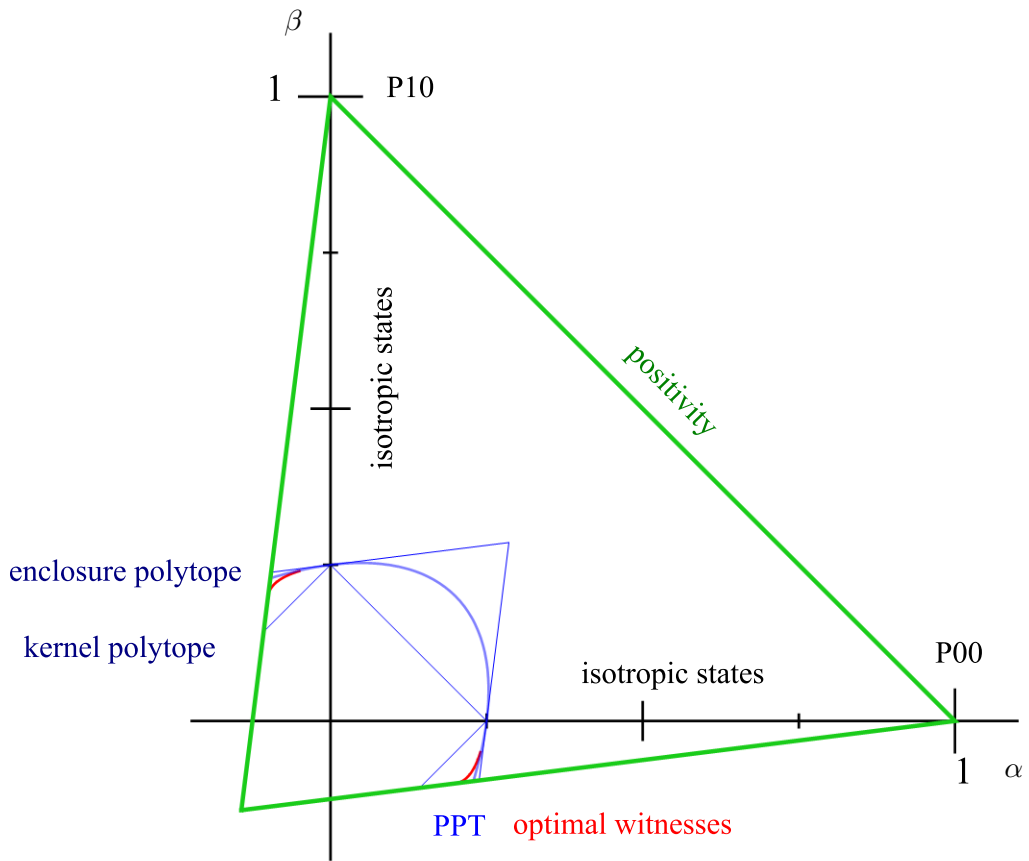
Figure 3.6: Illustration of the state $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$. All physical states lie within the green triangle which represents the border of positivity. The blue lines correspond to the enclosure polytope (the outer one) and the kernel polytope (the inner one). PPT states lie within the blue ellipse and there is also a small region of bound entanglement (region between the red curve given by optimal witnesses and the PPT boundary)
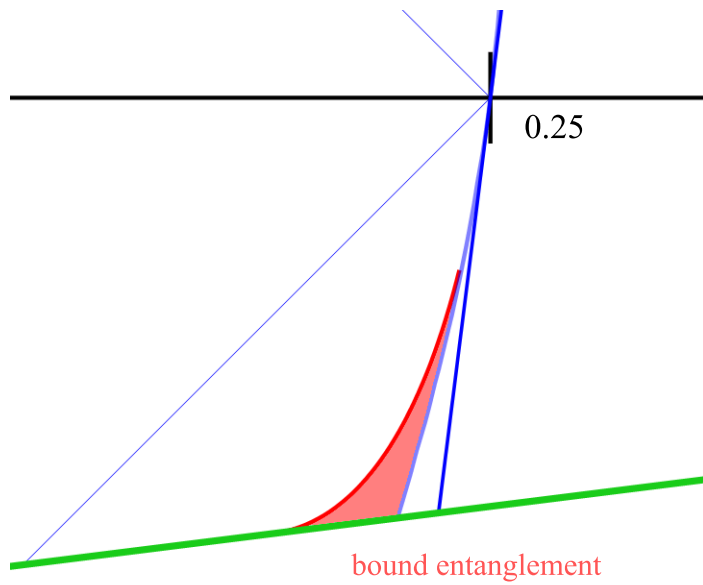

Figure 3.7: Enlarged illustration of the region of the state $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$ where bound entanglement appears (filled red)

Next, we consider three-parameter families of states of form $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{k,l} + \beta P_{m,n} + \gamma P_{p,q}$ with $k, l, m, n, p, q \in \{0, .., 2\}$. In section §3.2.2 it has been shown that for fixed parameters α, β, γ any state of this family is either locally unitarily equivalent to the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$ or $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{0,1}$ depending on whether the index pairs $\{(k, l), (m, n), (p, q)\}$ form a line or not. In both cases positivity restricts α, β, γ to lie within the region $\alpha \geq \frac{\beta+\gamma-1}{8}$ (and all parameter permutations of this term) and $\gamma \leq 1 - \alpha - \beta$. The PPT boundary for states on a line reads (see Appendix E)

$$(2\alpha + 2\beta + 2\gamma + 1)(8\alpha^2 + 8\beta^2 + 8\gamma^2 + 2\alpha + 2\beta + 2\gamma - 11\beta\alpha - 11\alpha\gamma - 11\beta\gamma - 1) = 0$$

and for states off a line we get (see Appendix F)

$$-16\alpha^3 - 16\beta^3 - 16\gamma^3 + 6\beta\alpha^2 + 6\gamma\alpha^2 + 6\gamma^2\alpha + 6\beta^2\alpha + 6\beta^2\gamma + 6\beta\gamma^2$$
$$-12\alpha^2 - 12\beta^2 - 12\gamma^2 + 3\beta\alpha + 3\gamma\alpha + 3\beta\gamma - 15\beta\gamma\alpha + 1 = 0 .$$

Like in the previous case, the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$ is invariant under horizontal reflection and for this reason the search for optimal witnesses can once again be restricted on $W = \frac{1}{3}\mathbb{1} + aP_{0,0} + bP_{1,0} + cP_{2,0}$ with $M_\phi = \mathbb{1} + aW_{0,0}|\phi\rangle\langle\phi|W_{0,0}^\dagger + bW_{1,0}|\phi\rangle\langle\phi|W_{1,0}^\dagger + cW_{2,0}|\phi\rangle\langle\phi|W_{2,0}^\dagger$. In [52] a choice for the parameters a, b, c in compliance with the constraints for optimal witnesses was found that yields

$$40\alpha^2 + (17\beta + 17\gamma - 14)\alpha + 4\beta^2 + \gamma(4\gamma - 5) - \beta(19\gamma + 5) + 1 = 0$$
$$\text{and permutations: } (\alpha \leftrightarrow \beta), (\alpha \leftrightarrow \gamma), (\beta \leftrightarrow \gamma)$$

for the boundary $Tr(W_{opt.}\rho) = 0$. Unfortunately, for states off a line there exists no such solution because obtaining it is much more difficult due to the fact that all nine parameters $\kappa_{k,l}$ of $W = \sum_{k,l}\kappa_{k,l}P_{k,l}$ have to be taken into account because the state has fewer symmetries. Regardless of this, for both states the boundaries of positivity and PPT are graphically illustrated in the following figures.
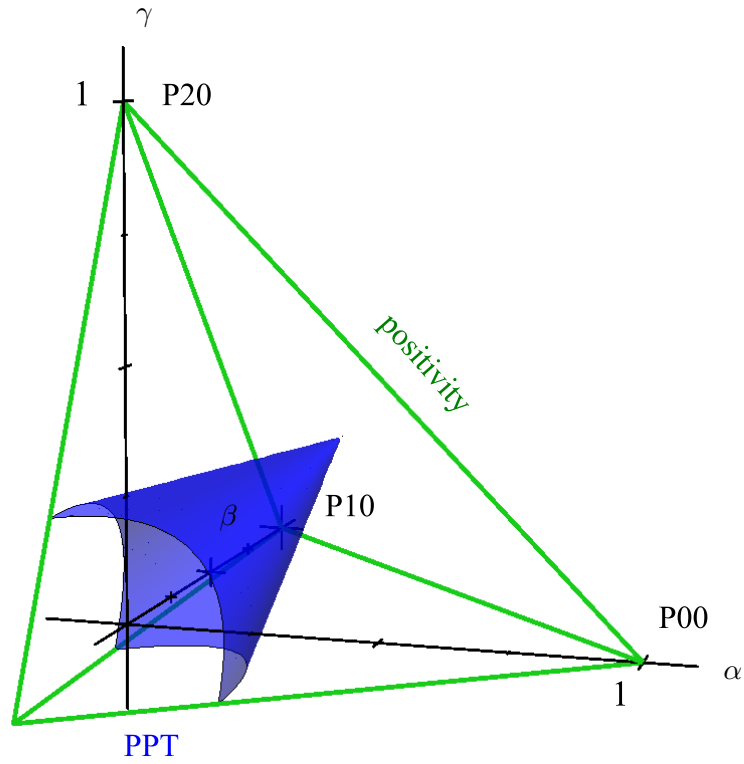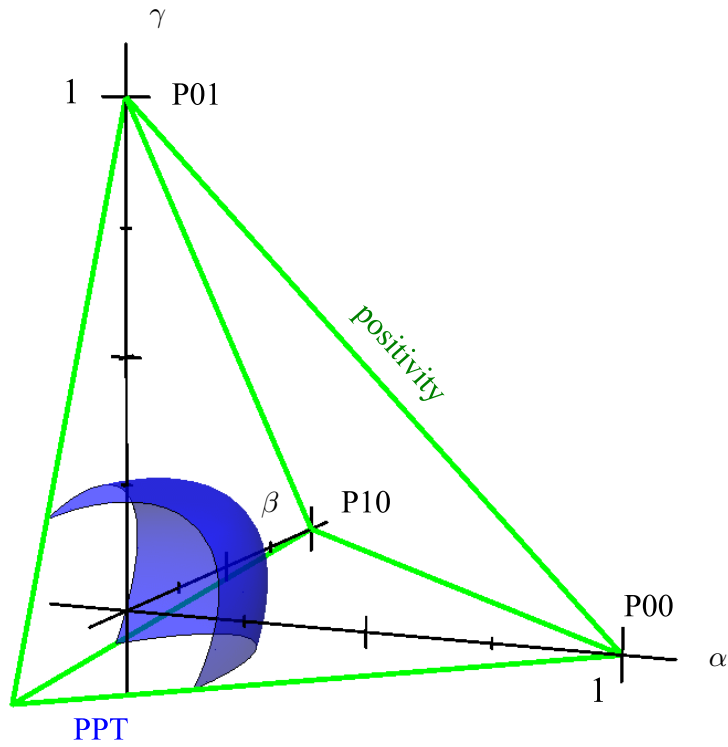
Figure 3.8: Illustration of the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$. Physical states lie within the green tetrahedron (positivity). The boundary of PPT states is a cone (blue) and thus all states beyond this surface are entangled. The tip of the cone touches the surface of positivity at $\alpha = \beta = \gamma = \frac{1}{3}$ illustrating the separability of the line state ρ_{line}

Figure 3.9: Illustration of the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{0,1}$. Physical states lie within the green tetrahedron (positivity). The surface of the PPT state region is a complex geometric object (blue surface)

3.2.4 Geometry of non-local states

Our purpose is to determine the set of states ρ of the magic simplex $\mathcal{W}$ that violate the CGLMP inequality. For any state of this kind there exists a Bell operator $\mathcal{B}_{I_d}$ such that $I_d = Tr(\rho \mathcal{B}_{I_d}) > 2$ and thus a state ρ for which the inequality $\max_{\mathcal{B}_{I_d}} Tr(\mathcal{B}_{I_d}) \leq 2$ holds is an element of the complementary set. This means that the complement and thereof the set itself can be determined by use of the optimisation procedure that has been introduced in §2.3.2. In general, it is computationally intensive to determine the boundary with high precision because states of $\mathcal{W}$ have to be parameterised and varied until a required precision ΔI of $\max I_d = \max_{\mathcal{B}_{I_d}} Tr(\mathcal{B}_{I_d}\rho) = 2 \pm \Delta I$ is reached. However, in the case when for a given state $\mu \in \mathcal{W}$ the maximal value of $\max I_d(\mu) = \max_{\mathcal{B}_{I_d}} Tr(\mathcal{B}_{I_d}\mu)$ is known with high accuracy it is not necessary to perform further numerical investigations in order to obtain the state on the boundary for the family $\rho = \frac{1-a}{d^2}\mathbb{1} + a\mu$ because of the relation $Tr(\mathcal{B}_{I_d}) = 0$ (see §2.3.1),

$$
\begin{aligned}
\max_{\mathcal{B}_{I_d}} Tr(\mathcal{B}_{I_d}\rho) &= \max_{\mathcal{B}_{I_d}} Tr(\mathcal{B}_{I_d}\left[\frac{1-a}{d^2}\mathbb{1} + a\mu\right]) \\
&= \max_{\mathcal{B}_{I_d}} Tr(\mathcal{B}_{I_d}a\mu) \\
&= a \max I_d(\mu) .
\end{aligned}
\tag{3.59}
$$

Hence, $\rho = \frac{1-a}{d^2}\mathbb{1} + a\mu$ lies on the boundary of (non-)locality for $a = 2/\max I_d(\mu)$. For our numerical investigations of the three families of states $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$, $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$ and $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{0,1}$ this fact is of great help because out of any numerical obtained value $\max I_3(\rho)$ we can derive a state on the boundary. More precisely, for a certain choice of α, β and γ[15] with resulting value $\max I_3(\rho)$ it implies that the state with the parameter values $\alpha_b = [2/\max I_3(\rho)] \cdot \alpha$, $\beta_b = [2/\max I_3(\rho)] \cdot \beta$ and $\gamma_b = [2/\max I_3(\rho)] \cdot \gamma$ lies on the boundary. For instance, the subsequent illustrations of the boundaries of (non-)locality were deduced from values $\max I_3(\rho)$ of states on the boundaries of positivity ($\alpha = \frac{\beta+\gamma-1}{8}$ (and all parameter permutations of this term) and $\gamma = 1-\alpha-\beta$). For the two-parameter family we calculated $\max I_3(\rho)$ for 60 such equally spaced points and for each of the two three-parameter families we calculated $\max I_3(\rho)$ for 920 of them.

---

[15]$\gamma=0$ for the first family $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$
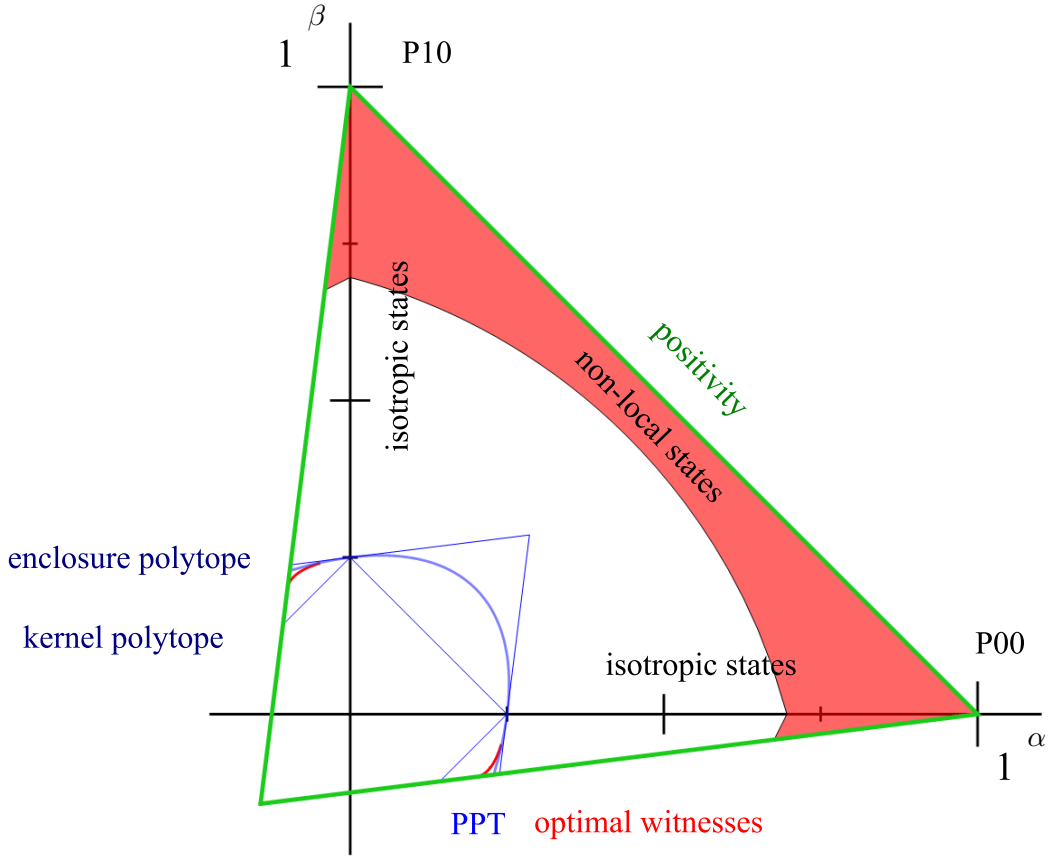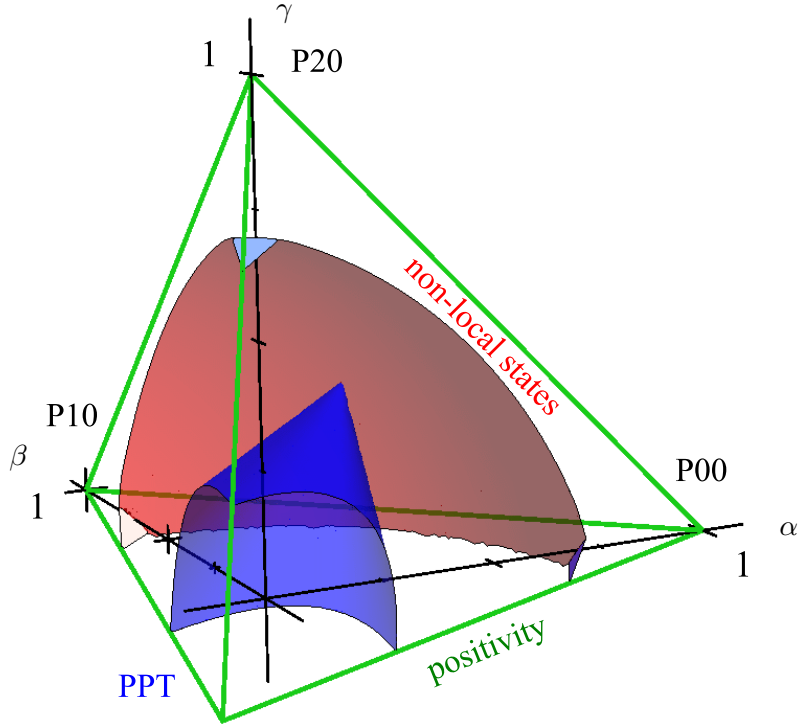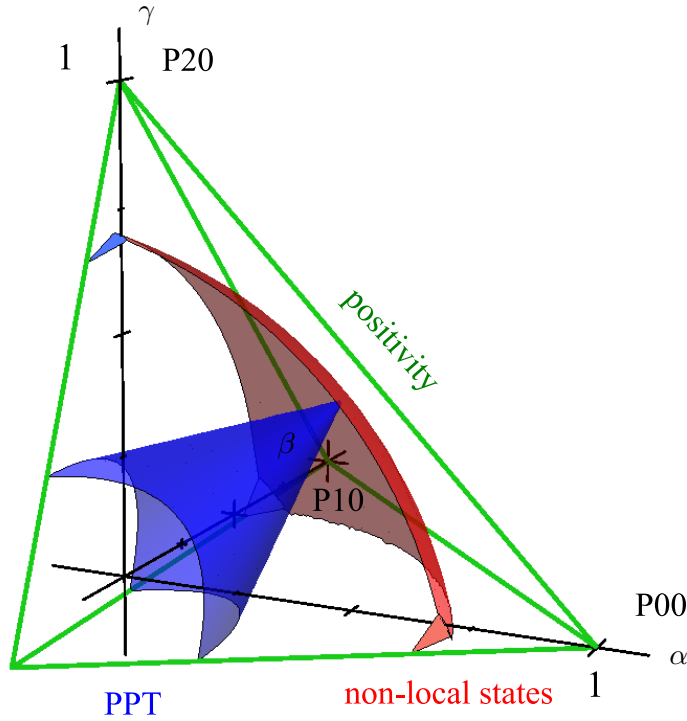
Figure 3.10: Illustration of the state $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$. All physical states lie within the green triangle which represents the border of positivity. States ρ in the red filled area violate the CGLMP inequality ($\max I_3(\rho) > 2$)

The result of the calculations for the state $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$ is illustrated in the above figure. The calculated points on the boundary are connected through lines and the area of non-local states is filled red. The boundary of (non-)locality seems to describe a circle for $\alpha, \beta > 0$ and a line if one of the parameters is negative, i.e. $\alpha < 0$ or $\beta < 0$. Suggestions on their specifications are given after the next figures illustrating the family $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$.

Figure 3.11: Illustration of the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$. States ρ beyond the red/blue shaded surface violate the CGLMP inequality $(\max I_3(\rho) > 2)$.

Figure 3.12: Illustration of the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$ form a different perspective. States ρ beyond the red/blue shaded surface violate the CGLMP inequality $(\max I_3(\rho) > 2)$.

The result of the calculations for the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$ is illustrated in the figures on the previous page. The calculated points on the boundary tendentially describe a spherical surface that is intersected by planes in the region of negative parameters. Based on symmetries and the facts that the boundaries of positivity, PPT and (non-)locality meet at the point $\alpha = \beta = \gamma = \frac{1}{3}$ and that the suggested analytical ideal measurements (2.49) yield the boundary parameter $\frac{1}{2}(6\sqrt{3} - 9)$ for the isotropic states, we were able to derive the radius $r = \frac{1}{156}(413\sqrt{3} - 558)$ and the center of the sphere $\alpha = \beta = \gamma = \frac{1}{156}(-361 + 186\sqrt{3})$. These specifications coincide with the numerical data up to the order 10^{-5} and we believe that these discrepancies should decrease for better accuracy and precision goals of the numerical optimisation (see §2.3.2). We suppose that the intersecting planes are given by the functions $\gamma = \frac{1}{2}(\alpha + \beta + 6\sqrt{3} - 9)$ (and permutations $\alpha \leftrightarrow \gamma$, $\beta \leftrightarrow \gamma$) because of compliance with the boundaries of the isotropic states and the numerical data (also up the order 10^{-5}). It should be noted that the circle and line boundaries in figure 3.10 can easily be obtained on the basis of these specifications because it solely illustrates the special case $\gamma = 0$.

For the remaining family $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{0,1}$ the geometric form of the boundary seems to be more complex and therefore we do not want to make any uncovered suggestions on the exact form. To get an impression of this, we have illustrated the raw data points in the following figures. Besides the complex shape of the boundary, we recognised an interesting peculiarity, namely, in contrast to the mixtures of states on a line where there is only one state $\alpha = \beta = \gamma = \frac{1}{3}$ on the boundary of positivity $1 - \alpha - \beta - \gamma = 0$ that does not violate the CGLMP inequality, here we have a whole region of local states for $1 - \alpha - \beta - \gamma = 0$. Moreover, in comparison the entire region of non-local states is smaller while the region of entangled states is larger. This can be seen as a further example for the diverging behaviour of these properties.
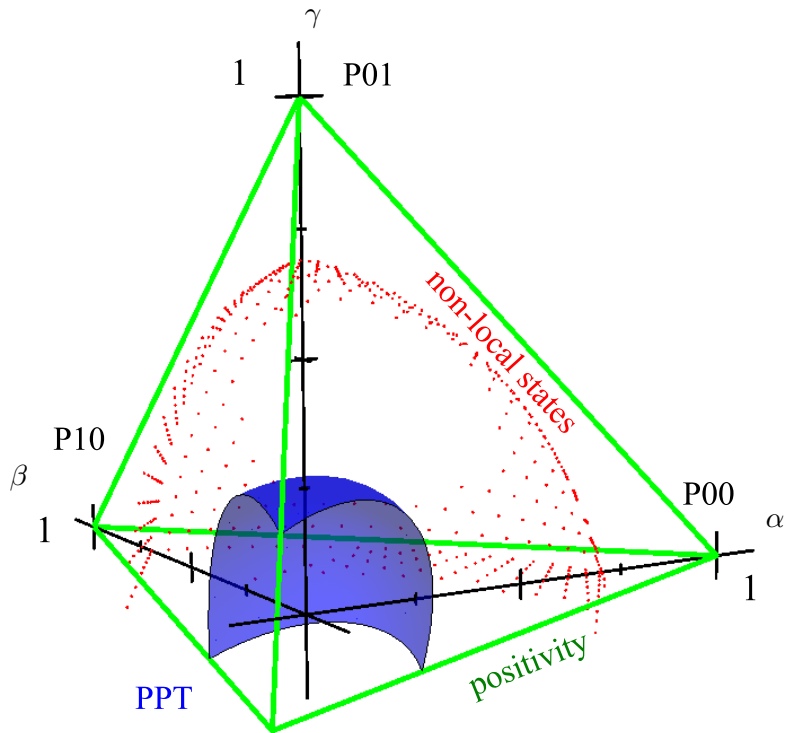
Figure 3.13: Illustration of the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{0,1}$. Red points denote states on the boundary of nonlocality ($\max I_3(\rho) = 2$).
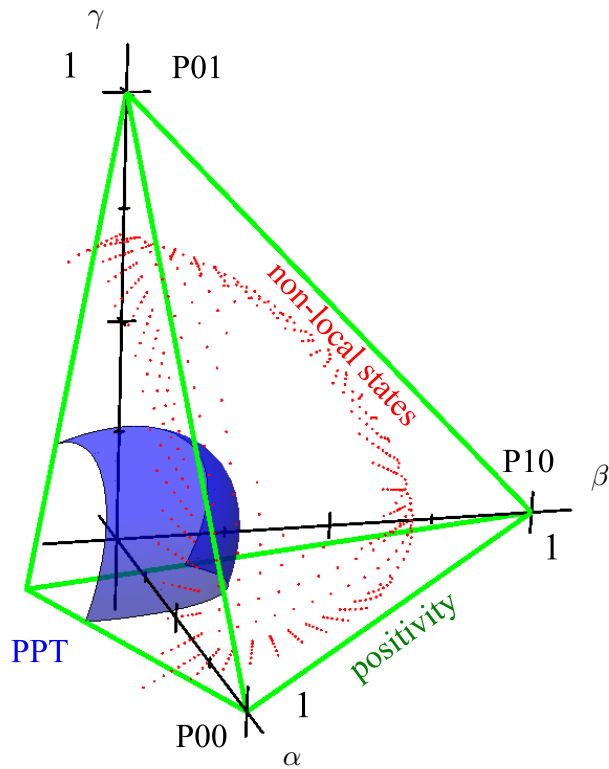

Figure 3.14: Illustration of the state $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{0,1}$. Red points denote states on the boundary of nonlocality ($\max I_3(\rho) = 2$).

3.3 Geometry of multipartite qubit systems (publication)

In this section we present a paper that was published on *Physical Review A 78* in collaboration with Beatrix Hiesmayr, Marcus Huber, Florian Hipp and Philipp Krammer. In this, we discuss a generalisation of the tetrahedron for multipartite qubit systems. We investigate separability, nonlocality and distillability with regard to a multipartite entanglement measure. In the context of this diploma thesis, this should be regarded as a further example of a geometric investigation of the state space. We emphasise that, because it contains several concepts for the study of multipartite systems that have not been introduced. Most of them should be self-explanatory or easily comprehensible with the knowledge gained in this thesis. Nonetheless, we recommend to read the cited publications.

Simplex of bound entangled multipartite qubit states

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We construct a simplex for multipartite qubit states of even number n of qubits, which has the same geometry concerning separability, mixedness, kind of entanglement, amount of entanglement, and nonlocality as the bipartite qubit states. We derive the entanglement of the class of states which can be described by only three real parameters with the help of a multipartite measure for all discrete systems. We prove that the bounds on this measure are optimal for the whole class of states and that it reveals that the states possess only n-partite entanglement and not, e.g., bipartite entanglement. We then show that this n-partite entanglement can be increased by stochastic local operations and classical communication to the purest maximal entangled states. However, pure n-partite entanglement cannot be distilled; consequently all entangled states in the simplex are n-partite bound entangled. We study also Bell inequalities and find the same geometry as for bipartite qubits. Moreover, we show how the (hidden) nonlocality for all n-partite bound entangled states can be revealed.

I. INTRODUCTION

Entanglement is at the heart of the quantum theory. It is the source of several new applications as quantum cryptography or a possible quantum computer. In recent years the study of higher-dimensional quantum systems and/or multipartite systems has shown that different aspects of the entanglement feature arise. They may have new applications such as multiparty cryptography.

In this paper we contribute to the classification of entanglement in a twofold way, i.e., which kind of entanglement a certain class of multipartite qubit states possesses, using the multipartite measure proposed in Ref. [1], and whether this kind of entanglement can be distilled. Our results suggest that for multipartite systems one can distinguish between different possibilities.

The class of states we analyze are a generalization of the class of states which form the well-known simplex for bipartite qubits (Sec. II), i.e., all locally maximally mixed states [2,3]. We make an obvious generalization and find an analogous simplex for states composed of an even number of qubits n, i.e., this class of states shows the same geometry concerning positivity, mixedness, separability, and entanglement (Sec. III). Further, the used multipartite measure [1] reveals that the kind of entanglement possessed is only n-partite entanglement where n is the number of qubits involved. The vertex states of the simplex are represented in the bipartite case by the well-known Bell states; for $n > 2$ they are equivalent to the generalized Smolin states proposed by Refs. [4,6–8].

Then we discuss the distillability of the entangled states and find states for which the n-partite entanglement can be increased by a protocol based only on copy states and stochastic local operations and classical communications (LOCC). We show that the state is not distillable for any subset of parties and hence bound entangled; however, the n-partite entanglement can be enhanced to reach the maximal possible purity and n-partite entanglement within the class of states under investigation, i.e., the vertex states. For a subset of these states it has been shown that they allow for quantum

information concentration (e.g., Refs. [4,5]), so we suggest that it might still be advantageous to enhance the n-partite bound entangled states for some applications.

Last but not least, in Sec. VI we address the question as to which of the simplex states violate the generalized Bell inequality which was shown to be optimal in this case, and draw its geometrical picture, Fig. 4.

II. THE SIMPLEX FOR BIPARTITE QUBITS

A single qubit state ω exists in a two-dimensional Hilbert space, i.e., $\mathcal{H} \equiv \mathbb{C}^2$, and any state can be decomposed into the well-known Pauli matrices σ_i:

$$\omega = \frac{1}{2}(\mathbb{1}_2 + n_i \sigma_i),$$

with the Bloch vector components $\vec{n} \in \mathbb{R}^3$ and $\Sigma_{i=1}^3 n_i^2 = |\vec{n}|^2 \leq 1$. For $|\vec{n}|^2 < 1$ the state is mixed (corresponding to $\mathrm{Tr}\,\omega^2 < 1$) whereas for $|\vec{n}|^2 = 1$ the state is pure ($\mathrm{Tr}\,\omega^2 = 1$).

The density matrix of two qubits ρ on $\mathbb{C}^2 \otimes \mathbb{C}^2$ is usually obtained by calculating its elements in the standard product basis, i.e., $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$. Alternatively, we can write any two-qubit density matrix in a basis of 4×4 matrices, the tensor products of the identity matrix $\mathbb{1}_2$, and the Pauli matrices,

$$\rho = \frac{1}{4}(\mathbb{1}_2 \otimes \mathbb{1}_2 + a_i \sigma_i \otimes \mathbb{1}_2 + b_i \mathbb{1}_2 \otimes \sigma_i + c_{ij} \sigma_i \otimes \sigma_j)$$

with $a_i, b_i, c_{ij} \in \mathbb{R}$. The parameters a_i and b_i are called *local* parameters as they determine the statistics of the reduced matrices, i.e., of Alice's or Bob's system. In order to obtain a geometrical picture one considers in the following only states where the local parameters are zero ($\vec{a} = \vec{b} = \vec{0}$), i.e., the set of all locally maximally mixed states, $\mathrm{Tr}_A(\rho) = \mathrm{Tr}_B(\rho) = \frac{1}{2}\mathbb{1}_2$ (see also Refs. [2,3]).

A state is called separable if and only if it can be written in the form $\Sigma_i p_i \rho_i^A \otimes \rho_i^B$ with $p_i \geq 0$, $\Sigma p_i = 1$, otherwise it is entangled. As the property of separability does not change under local unitary transformation and classical communica-
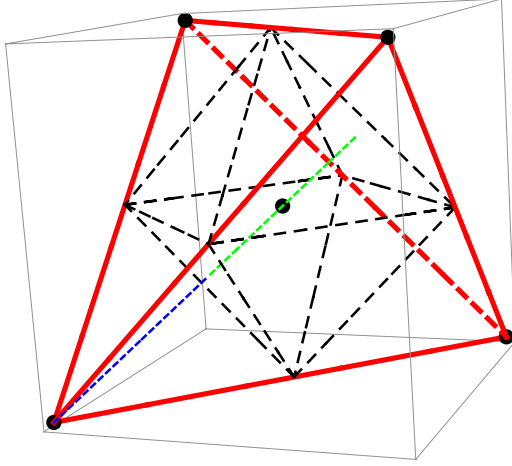
FIG. 1. (Color online) Here the geometry of the state space of even number of qubits is visualized. Each state is represent by a triple of three real numbers $\vec{c}$, Eq. (1). The four black dots at the vertices of the cube represent four orthogonal "vertex" states. In the case of two qubits these are the four maximally entangled Bell states $\psi^{\pm}, \phi^{\pm}$ and for higher n they are equal mixtures of $2^n/4$ Greenberger-Horne-Zeilinger (GHZ) states. The positivity condition forms a tetrahedron (red) with the four "vertex" states and the totally mixed state at the origin (black dot in the middle). All separable states are represented by points inside and at the surface of the octahedron (dashed object). The dashed line represents for $n=2$ the Werner states and for $n>2$ the generalized Smolin states (becoming separable when blue changes into green).

tion, the states under consideration can be written in the form [2]

$$\rho = \frac{1}{4}(\mathbb{1}_2 \otimes \mathbb{1}_2 + c_i \sigma_i \otimes \sigma_i),$$

where the c_i are three real parameters and can be considered as a vector $\vec{c}$ in Euclidean space. Differently stated, for any locally maximally mixed state ρ the action of two arbitrary unitary transformations $U_1 \otimes U_2$ can via the homomorphism of the groups SU(2) and SO(3) be related to unique rotations $O_1 \otimes O_2$. Thus the correlation matrix $c_{ij}\sigma_i \otimes \sigma_j$ can be chosen such that the matrix c_{ij} gets diagonal via singular value decomposition. Therefore, three real numbers combined to a vector $\vec{c}$ can be taken as representative of the state itself.

In Fig. 1 we draw the three-dimensional picture, where each point $\vec{c}$ corresponds to a locally maximally mixed state ρ. The origin $\vec{c}=\vec{0}$ corresponds to the totally mixed state, i.e., $\frac{1}{4}\mathbb{1}_2 \otimes \mathbb{1}_2$. The only pure states in the picture are given by $|\vec{c}|^2 = 3$ and represent the four maximally entangled Bell states $|\psi^{\pm}\rangle = (1/\sqrt{2})\{|01\rangle \pm |10\rangle\}$, $|\phi^{\pm}\rangle = (1/\sqrt{2})\{|00\rangle \pm |11\rangle\}$, which are located at the vertices of the cube. The planes spanned by these four points are equivalent to the positivity criterion of the state ρ. Therefore, all points inside the tetrahedron represent the state space.

It is well known that density matrices which have at least one negative eigenvalue after partial transpose (PT) are entangled. The inversion of the argument is true only for systems with $2\otimes2$ and $2\otimes3$ degrees of freedom. The PT corresponds to a reflection, i.e., $c_2 \to -c_2$ with all other components unchanged. Thus all points inside and at the surface of the octahedron represent all separable states in the set. Of course, one can always make the transformation $\vec{c} \to -\vec{c}$, and thus one obtains a mirrored tetrahedron, spanned by the four other vertices of the cube. Clearly, the intersection of these two tetrahedra contain all states which have positive eigenvalues after the action of the PT.

In Ref. [9–11] a generalization to higher-dimensional bipartite states is considered and a so-called magic simplex for qudits is obtained. Here the class of all locally maximally mixed states have to be reduced in order to obtain this generalized simplex. Already for bipartite qutrits many new symmetries arise and regions of bound entanglement can be found (see also Refs. [12–16]).

We also want to generalize the simplex of bipartite qubits; however, in our case we increase the number of qubits.

III. A SIMPLEX FOR *n*-PARTITE QUBIT STATES

Assume we have n qubits. Then a generalization can be written as

$$\rho = \frac{1}{2^n}\left(\mathbb{1} + \sum c_i \sigma_i \otimes \sigma_i \otimes \cdots \otimes \sigma_i\right) := \frac{1}{2^n}\left(\mathbb{1} + \sum c_i \sigma_i^{\otimes n}\right). \tag{1}$$

Obviously, for this generalization we follow the strategy to set the local parameters of all subsystems j, $\mathrm{Tr}_{1,2,\ldots,j-1,j+1,\ldots,n}(\rho)$, to zero, as well as the parameters shared by two parties j,k, $\mathrm{Tr}_{1,2,\ldots,j-1,j+1,\ldots,k-1,k+1,\ldots,n}(\rho)$, zero and so on until $n-1$ zero.

Again the state can be represented by a three-dimensional vector $\vec{c}$. For $n=3$ the positivity condition $\rho \geq 0$ requires[1]

$$|\vec{c}|^2 \leq 1. \tag{2}$$

This turns out to be the case for all odd numbers of qubits involved.

For even numbers of qubits the positivity condition $\rho \geq 0$ requires that the vector is within the following four planes:[2]

$$1 + \vec{c} \cdot \vec{n}^{(i)} \geq 0 \quad \text{with} \quad \vec{n}^{(i)}$$

$$= \begin{pmatrix} -1 \\ +1 \\ +1 \end{pmatrix}, \quad \begin{pmatrix} +1 \\ -1 \\ +1 \end{pmatrix}, \quad \begin{pmatrix} +1 \\ +1 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix}. \tag{3}$$

These conditions are exactly the same ones as for the two-qubit case $n=2$, i.e., the four planes above form the magic tetrahedron.

---

[1] The result is obtained by using a standard computer programm.
[2] Note that for $n=4,8,\ldots$ the mirrored tetrahedron ($\vec{c} \to -\vec{c}$) is obtained. Again the result is obtained by using a standard computer programm.

The purity $\text{Tr}(\rho^2)$ gives $(1/2^n)(1+|\vec{c}|^2)$; thus the states with $|\vec{c}|^2=3$ are the purest states of the class of states under investigation and are located in the vertices of the tetrahedron. Note that with increasing n the percentage of purity decreases, i.e., only for $n=2$ do the vertices present pure states. Further analysis of these vertex states follows later.

Now we want to investigate if the separability condition also for $n>2$ corresponds to the octahedron. The partial transpose of one qubit ($\text{PT}_{\text{one qubit}}$) changes the sign in front of the $\sigma_2^{\otimes n}$ matrix, i.e., the y component of the vector $\vec{c}$ changes sign. Therefore the states under investigation are entangled by the necessary but not sufficient (one-qubit) Peres criterion

$$n=3,5,\ldots, \quad |\vec{c}|^2 \leq 1,$$

$$n=2,4,\ldots, \quad 1-\vec{c}\cdot\vec{n}^{(i)} \leq 0. \tag{4}$$

Taking the partial transpose of two, four, …qubits changes two, four, …times the sign and consequently one obtains the positivity criterion (3). Taking the partial transpose of odd qubits is equivalent to $\text{PT}_{\text{one qubit}}$.

For even number of qubits the above Peres criterion implies a mirrored tetrahedron, analogously to the bipartite case; however, we do not know if the intersection, the octahedron, contains only separable states. For odd numbers of qubits the situation is different and we will not investigate it further.

Now two questions arise: first, are all states represented by the octahedron separable and, second, what kind of entanglement does this class of states possess?

Let us tackle the second question first. To analyze our generalized states ρ further we use the multipartite entanglement measure for all discrete systems introduced by Ref. [1]. The main idea is that the information content of any n-partite quantum system of arbitrary dimension can be separated in the following form:

$$\underbrace{I(\rho)+R(\rho)}_{\text{single property}}+\underbrace{E(\rho)}_{\text{entanglement}}=n \tag{5}$$

where

$$I(\rho) := \sum_{s=1}^{n} \underbrace{\mathcal{S}_s^2(\rho)}_{\text{single property of subsystem } s} \tag{6}$$

contains all locally obtainable information (i.e., obtainable information a party can measure on its particle), $E(\rho)$ contains all information encoded in entanglement, and $R(\rho)$ is the complementing missing information, due to a classical lack of knowledge about the quantum state. The total amount of entanglement $E(\rho)$ can be separated into m-flip concurrences by rewriting the linear entropy of all subsystems in an operator sum; thus one obtains

$$E(\rho) := \underbrace{\mathbf{C}_{(2)}^2(\rho)}_{\text{two-flip concurrence}} + \underbrace{\mathbf{C}_{(3)}^2(\rho)}_{\text{three-flip concurrence}} + (\cdots)$$
$$+ \underbrace{\mathbf{C}_{(n)}^2(\rho)}_{n\text{-flip concurrence}}. \tag{7}$$

These m-flip concurrences are useful for two reasons: first, one can obtain bounds on the operators and thus handle mixed states and, second, the authors of Ref. [1] showed (for three qubits) that the m-flip concurrences can be reordered such that they give the m-partite entanglement, which in addition coincides with the m-separability [17].

Here we extend their result for the states under investigation. Due to the high symmetry of the class of states under investigation the bounds of the m-partite entanglement can be computed and herewith we can reveal the following substructure of total entanglement $E(\rho)$,

$$E(\rho) = \underbrace{E_{(2)}(\rho)}_{\text{bipartite entanglement}} + \underbrace{E_{(3)}(\rho)}_{\text{tripartite entanglement}}$$
$$+ \cdots + \underbrace{E_{(n)}(\rho)}_{n\text{-partite entanglement}} \tag{8}$$

with the subsubstructure

$$E_{(2)}(\rho) = E_{(12)}(\rho) + E_{(13)}(\rho) + \cdots + E_{(1n)}(\rho) + E_{(23)}(\rho) + \cdots$$
$$+ E_{(2n)}(\rho) + \cdots + E_{(n-1,n)}(\rho),$$

$$E_{(3)}(\rho) = E_{(123)}(\rho) + \cdots + E_{(n-2,n-1,n)}(\rho),$$

$$\cdots = \cdots$$

$$E_{(n)}(\rho) = E_{(12\cdots n)}(\rho). \tag{9}$$

We find that for the states under investigation the only non-vanishing entanglement is the n-partite entanglement and it becomes (for details, see Sec. IV)

$$E_{(n)} = E_{12,\ldots,n} = X \max\left(0, \frac{1}{2}\max(-1+\vec{c}\cdot\vec{n}^{(1)}, -1+\vec{c}\cdot\vec{n}^{(2)}, \right.$$
$$\left. -1+\vec{c}\cdot\vec{n}^{(3)}, -1+\vec{c}\cdot\vec{n}^{(4)})\right)^2, \tag{10}$$

where $X=1$ except for bipartite qubits, when it is $X=2$ (the reason for this difference is explained later). Hence, we find the same condition for being entangled as given by the one-qubit Peres criterion.

Now, if these bounds are exact also for $n>2$, then all states represented by the octahedron are separable. Indeed, it turns out that this is the case. We give the proof of separability separately in the Appendix.

In summary, we have found for an even number of qubits the same geometry as in the case of bipartite qubits, also depicted by Fig. 1. Moreover, we have shown that the multipartite entanglement measure proposed by Ref. [1] works tightly as the bounds are exact and it reveals only n-partite entanglement. Let us discuss this result more carefully.

For the purest states, $|\vec{c}|^2=3$, located in the vertices of the tetrahedron, the maximal n-partite entanglement results as $E_{(n)}=1$ except for $n=2$ when it is $E_{(n)}=2$. Thus the amount of entanglement for $n>2$ is independent of the number of qubits involved. The reason for the difference can be found in the information content of the multipartite system, Eq. (5). The maximal entanglement of an n-partite state is n. This is the case if and only if the local obtainable information of all subsystems is zero and the classical lack of knowledge of the quantum state is also zero, i.e., the total state is also pure. For bipartite qubits, $n=2$, the vertex states are the Bell states, which have maximal entanglement 2 whereas the locally obtainable information S is zero, as well as the lack of classical knowledge about the quantum state $R=0$.

By construction for $n>2$ we set the locally obtainable information S of all subsystems to zero; however, also all possible locally obtainable information shared by two, three, ..., $n-1$ parties is set to zero; obviously this is not compatible with being maximally entangled. The information content for $n>2$ is given by

$$n = E_n + R = 1 + R, \tag{11}$$

and consequently the lack of classical knowledge is nonzero, i.e., $R=n-1$. Differently stated for $n=4$, any party has the trace state and also any two parties and any three parties share the trace state, therefore $R=3$.

Remark. The local information $S_s(\rho)$ of one subsystem s is nothing else than Bohr's quantified complementarity relation [18–20], with its well-known physical interpretation in terms of predictability and visibility (coherence). One can extend this concept for two parties sharing a state; then the (bi)local information of total multipartite system can be defined in similar way and is complemented by the mixedness of the shared bipartite system. Again this (bi)local information is obtainable only if and only if the state is not the trace state.

Coming back to the simplex geometry we see that the closer we get to the origin the more the amount of entanglement is reduced by increasing the amount of classical uncertainty R only.

For bipartite qubits the vertex states $|\vec{c}|^2=3$ are the four Bell states. For n qubits we find for $|\vec{c}|^2=3$ also four unitary equivalent states; however, they are no longer pure. For $n=4$ the state is an equally weighted mixture of four $|GHZ\rangle$ states. Starting with one GHZ state, e.g.,

$$|GHZ\rangle = \frac{1}{\sqrt{2}}\{|0000\rangle + |1111\rangle\}, \tag{12}$$

one obtains another representation by applying two flips, i.e., $\mathbb{1}\otimes\mathbb{1}\otimes\sigma_x\otimes\sigma_x$, and then applying on the new GHZ state rep-

resentation the operator $\mathbb{1}\otimes\sigma_x\otimes\sigma_x\otimes\mathbb{1}$, and onto that new GHZ state representation the operator $\sigma_x\otimes\sigma_x\otimes\mathbb{1}\otimes\mathbb{1}$, giving the last GHZ state representation. The other three vertex states are obtained by applying only one Pauli matrix. For $n=6$ we have 2^6 GHZ states where $2^6/4$ GHZ states equally mix for one vertex state.

Remark. We find the same symmetry for the bipartite qubit case, one Bell state is mapped into another by one Pauli matrix; however, applying two Pauli matrices maps a Bell state onto itself, therefore we have no mixture of different maximally entangled states.

In the next section we give the detailed calculation of the measure and in the following section we investigate the question whether the entangled states are bound entangled and if so in what sense their entanglement is bound. In particular we discuss what it means that the substructure revealed by the measure shows only n-partite entanglement.

IV. DERIVATION OF THE MULTIPARTITE MEASURE FOR THE SIMPLEX STATES

In Ref. [1] a multipartite measure for multidimensional systems as a kind of generalization of Bohr's complementarity relation was derived. Here, we give explicitly the results for $n=2$ and 4 expressed in the familiar Pauli matrix representation

It is well known that to compute the concurrence introduced by Hill and Wootters [21] one has to consider

$$\rho(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y) \tag{13}$$

where the complex conjugation is taken in the computational basis. The concurrence is then given by the formula

$$\mathcal{C} = \max\{0, 2\max\{\lambda_1,\lambda_2,\lambda_3,\lambda_4\} - (\lambda_1+\lambda_2+\lambda_3+\lambda_4)\} \tag{14}$$

where the λ_i's are the square roots of the eigenvalues of the above matrix. To obtain the information content we have to multiply this measure by 2.

The first observation in Ref. [1] is that the linear entropy, $M(\rho)=\frac{2}{3}[1-\mathrm{Tr}(\rho^2)]$ can be rewritten using operators. This means, e.g., for any pure four-qubit state,

$$|\psi\rangle = \sum_{i,j,k,l=0}^{1} a_{ijkl}|ijkl\rangle, \tag{15}$$

the linear entropy of one subsystem can be written as

$$M^2(\mathrm{Tr}_{234}|\psi\rangle\langle\psi|) = M^2(\rho_1) = \sum_{k,l=0}^{1}\sum_{\{i_1\neq i_1'\};\{i_2\neq i_2'\}} |\langle\psi|(\sigma_x\otimes\sigma_x\otimes\mathbb{1}\otimes\mathbb{1})(|i_1i_2kl\rangle\langle i_1i_2kl| - |i_1'i_2'kl\rangle\langle i_1'i_2'kl|)|\psi^*\rangle|^2$$

$$+ \sum_{k,l=0}^{1}\sum_{\{i_1\neq i_1'\};\{i_3\neq i_3'\}} |\langle\psi|(\sigma_x\otimes\mathbb{1}\otimes\sigma_x\otimes\mathbb{1})(|i_1ki_3l\rangle\langle i_1ki_3l| - |i_1'ki_3'l\rangle\langle i_1'ki_3'l|)|\psi^*\rangle|^2$$

$$+ \sum_{k,l=0}^{1} \sum_{\{i_1 \neq i_1'\};\{i_3 \neq i_3'\}} |\langle \psi|(\sigma_x \otimes 1 \otimes 1 \otimes \sigma_x)(|i_1kli_4\rangle\langle i_1kli_4| - |i_1'kli_3'\rangle\langle i_1'kli_4'|)|\psi^*\rangle|^2$$

$$+ \sum_{k,l=0}^{1} \sum_{\{i_2 \neq i_2'\};\{i_3 \neq i_3'\}} |\langle \psi|(1 \otimes \sigma_x \otimes \sigma_x \otimes 1)(|ki_2i_3l\rangle\langle ki_2i_3l| - |ki_2'i_3'l\rangle\langle ki_2'i_3'l|)|\psi^*\rangle|^2$$

$$+ \sum_{k,l=0}^{1} \sum_{\{i_2 \neq i_2'\};\{i_4 \neq i_4'\}} |\langle \psi|(1 \otimes \sigma_x \otimes 1 \otimes \sigma_x)(|ki_2li_4\rangle\langle ki_2li_4| - |ki_2'li_4'\rangle\langle ki_2'li_4'|)|\psi^*\rangle|^2$$

$$+ \sum_{k,l=0}^{1} \sum_{\{i_3 \neq i_3'\};\{i_4 \neq i_4'\}} |\langle \psi|(1 \otimes 1 \otimes \sigma_x \otimes \sigma_x)(|kli_3i_4\rangle\langle kli_3i_4| - |kli_3'i_4'\rangle\langle kli_3'i_4'|)|\psi^*\rangle|^2$$

$$+ \sum_{k}^{1} \sum_{\{i_1 \neq i_1'\};\{i_2 \neq i_2'\};\{i_3 \neq i_3'\}} |\langle \psi|(\sigma_x \otimes \sigma_x \otimes \sigma_x \otimes 1)(|i_1i_2i_3k\rangle\langle i_1i_2i_3k| - |i_1'i_2'i_3'k\rangle\langle i_1'i_2'i_3'k|)|\psi^*\rangle|^2$$

$$+ \sum_{k=0}^{1} \sum_{\{i_1 \neq i_1'\};\{i_2 \neq i_2'\};\{i_4 \neq i_4'\}} |\langle \psi|(\sigma_x \otimes \sigma_x \otimes 1 \otimes \sigma_x)(|i_1i_2ki_4\rangle\langle i_1i_2ki_4| - |i_1'i_2'ki_4'\rangle\langle i_1'i_2'ki_4'|)|\psi^*\rangle|^2$$

$$+ \sum_{k=0}^{1} \sum_{\{i_1 \neq i_1'\};\{i_3 \neq i_3'\};\{i_4 \neq i_4'\}} |\langle \psi|(\sigma_x \otimes 1 \otimes \sigma_x \otimes \sigma_x)(|i_1ki_3i_4\rangle\langle i_1ki_3i_4| - |i_1'ki_3'i_4'\rangle\langle i_1'ki_3'i_4'|)|\psi^*\rangle|^2$$

$$+ \sum_{k=0}^{1} \sum_{\{i_2 \neq i_2'\};\{i_3 \neq i_3'\};\{i_4 \neq i_4'\}} |\langle \psi|(1 \otimes \sigma_x \otimes \sigma_x \otimes \sigma_x)(|ki_2i_3i_4\rangle\langle ki_2i_3i_4| - |ki_2'i_3'i_4'\rangle\langle ki_2'i_3'i_4'|)|\psi^*\rangle|^2$$

$$+ \sum_{\{i_1 \neq i_1'\};\{i_2 \neq i_2'\};\{i_3 \neq i_3'\};\{i_4 \neq i_4'\}} |\langle \psi|(\sigma_x \otimes \sigma_x \otimes \sigma_x \otimes \sigma_x)(|i_1i_2i_3i_4\rangle\langle i_1i_2i_3i_4| - |i_1'i_2'i_3'i_4'\rangle\langle i_1'i_2'i_3'i_4'|)|\psi^*\rangle|^2, \quad (16)$$

where, e.g., $\{i_1\} \neq \{i_1'\}$, $\{i_2\} \neq \{i_2'\}$ means that the set of indices are not the same, i.e., the sum is taken over

$$\{i_1,i_2;i_1',i_2'\} = \{0,1;0,0\},\{0,0;0,1\},\{0,1;1,0\},\{0,0;1,1\},\{1,1;0,0\},\{1,0;0,1\},\{1,1;0,0\},\{1,0;0,1\},$$

$$\{0,0;1,0\},\{1,0;0,0\},\{0,0;1,1\},\{1,0;0,1\},\{0,1;1,0\},\{1,1;0,0\},\{0,1;1,1\},\{1,1;0,1\}. \quad (17)$$

Likewise the linear entropies for the other subsystem can be derived, i.e., separated into terms where the flip operator σ_x is applied two, three, or four times. It is well known that for pure states the sum over the entropies of all reduced density matrices is an entanglement measure; therefore using the linear entropy we get the following entanglement measure:

$$E(|\psi\rangle) := \sum_{s=1}^{4} M^2(\rho_s) = \sum_{m=2}^{4} [C^m(\psi)]^2, \quad (18)$$

where $(C^m)^2$ is the sum of all terms of all reduced matrices that contain m-flip operators. These quantities were called (squared) m-concurrences, because they play a similar role as the Wootters concurrence.

For mixed states ρ the infimum of all possible decompositions is an entanglement measure

$$E(\rho) = \inf_{p_i,|\psi_i\rangle} \sum_{p_i,|\psi_i\rangle} p_i E(|\psi_i\rangle). \quad (19)$$

The problem of the whole entanglement theory is that this infimum can in general not be calculated. Now we bring the operator representation of the linear entropy into the game, because for operators upper bounds can be obtained.

Let us start with the calculation of the four-flip concurrence $C^{(4)}$, which is the sum of all terms containing four-flips of the entropies of all reduced matrices, i.e.,

$$[C^{(4)}(\rho)]^2 = \inf_{p_i,|\psi_i\rangle} \sum_{p_i,|\psi_i\rangle} p_i [C^{(4)}(\psi_i)]^2. \quad (20)$$

As shown in Ref. [1] one can derive bounds on the above expression for any m-flip concurrence by defining, in an analogous way to the Hill and Wootters flip density matrix [21], the m-flip density matrix

$$\tilde{\rho}_s^m = O_s(|\{i_n\}\rangle\langle\{i_n\}| - |\{i_n'\}\rangle\langle\{i_n'\}|)\rho^*$$
$$\times O_s(|\{i_n\}\rangle\langle\{i_n\}| - |\{i_n'\}\rangle\langle\{i_n'\}|) \quad (21)$$

and calculating the λ_m^s's which are the squared roots of the eigenvalues of $\tilde{\rho}_s^m \rho$. The bound $B^{(m)}$ of the m-flip concurrence $C^{(m)}$ is then given by

$$B^m(\rho) := \left(\sum_s \max\left[0, 2 \max(\{\lambda_m^s\}) - \sum \{\lambda_m^s\} \right]^2 \right)^{1/2}.$$
(22)

From Eq. (16) we see that for the four-flip concurrence of subsystem ρ_1 four different operators occur, thus we have in total 16 different operators listed in Appendix B.

Inserting our class of states we find that for each operator $\mathcal{O}^s$ the eigenvalues are the same, i.e., one obtains eight zeros and the remaining four eigenvalues are exactly equivalent to the Peres criterion Eq. (4).

The same procedure has to be applied to calculate the three-flip and the two-flip concurrence. As can be seen from Eq. (16) here the unity and σ_z matrices are involved which lead to no contribution for the states under investigation. Remember that they are mixtures of the vertex states, which are equal mixtures of such GHZ states that differ by two flips. Therefore the total entanglement is given by the $C^{(4)}$ concurrence only and is a four-partite entanglement. For $n = 6, 8, \ldots$ the scenario is the same, because of the same underlying symmetry.

In Appendix A we show that all states not detected by the measure are separable; thus the bounds are optimal and therefore the measure detects all bound entangled states.

V. ARE THE ENTANGLED STATES BOUND ENTANGLED?

In Refs. [4,6–8] the special states $c = c_1 = -c_2 = c_3$ for $n > 2$, which were named generalized Smolin states (for $n = 2$ these states are the Werner states), are investigated and they show that for $1 \geq c > \frac{1}{3}$ these states are bound entangled. In particular, the authors argued that these states are bound entangled, because the states are separable against bipartite symmetric cuts like $12|34\ldots$, $14|23\ldots,\ldots$ and therefore no Bell state between any two subsystem can be distilled. This is obviously also the case for the whole class of states under investigation.

As the considered measure of entanglement revealed only n-partite entanglement and, e.g., not, m-partite entanglement ($m < n$), it may not seem directly obvious that Bell states (bipartite entanglement) cannot be distilled, because the class of states does not possess any bipartite entanglement. Thus the question could be refined to ask whether n-partite pure entanglement can be distilled.

For the n-partite class of states under investigation we consider a similar distillation protocol as the recurrence protocol by Bennett *et al.* [22]. For that we generalize it such that each party gets a copy onto which a unitary bilateral XOR operation is performed and afterward a measurement in, say, the z direction, is performed. Only states are kept where all parties found their copy qubit in say, the, up direction. This protocol favors, as do, all protocols one state; in our case for $n = 2$ it is the Φ^+ state and for $n > 2$ its equivalents.

In detail it goes as follows. We consider one state and its copy

$$\rho^{\otimes 2} = \left(\frac{1}{2^n} \{ \mathbb{1}^{\otimes n} + c_i \sigma_i^{\otimes m} \} \right)^{\otimes 2}$$
(23)

and all parties get a copy state. Therefore, we reorder the state by a unitary transformation such that the first and sec-
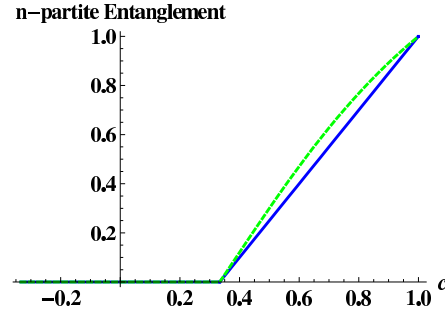

FIG. 2. (Color online) n-partite entanglement of the Werner states $n = 2$ (here the y axis has to be multiplied by 2) or the generalized Smolin states $n > 2$ before and after the application of the introduced protocol (upper dashed green curve). Note that the vertex states are mapped onto themselves by the given protocol.

ond terms in the tensor product belongs to Alice and the third and fourth terms to Bob, and so on:

$$\rho^{\otimes 2} \to \left(\frac{1}{2^n} \right)^2 [(\mathbb{1} \otimes \mathbb{1})^{\otimes n} + c_i (\mathbb{1} \otimes \sigma_i)^{\otimes n} + c_i (\sigma_i \otimes \mathbb{1})^{\otimes n}$$
$$+ c_i c_j (\sigma_i \otimes \sigma_j)^{\otimes n}].$$
(24)

Now each party performs on its two subsystems a unitary XOR operation

$$U_{\text{XOR}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
(25)

and then projects on the copy subsystem with $P = \frac{1}{2}(\mathbb{1} + \sigma_z)$. This gives again a state in the class of states under investigation, i.e., one finds

$$\vec{c} = \begin{pmatrix} c_x \\ c_y \\ c_z \end{pmatrix} \to \vec{c}_{\text{dis}} = \begin{pmatrix} \dfrac{c_x^2 + c_y^2}{1 + c_z^2} \\ \dfrac{2 c_x c_y}{1 + c_z^2} \\ \dfrac{2 c_z}{1 + c_z^2} \end{pmatrix}.$$
(26)

Comparing with the separability condition and with the positivity condition, one verifies that only separable states are mapped into separable states.

Let us consider the Werner states and the generalized Smolin states ($c = c_x = c_y = c_z$), for which we derive that the n-partite entanglement is always increased after the above protocol (see Fig. 2). For $-1/\sqrt{3} \leq c \leq 1/3$ the measure before and after the protocol is zero and for $c = 1$ the state is mapped onto itself. For $1/3 < c < 1$ the entanglement of the distilled state is increased compared to the input state. In Fig. 3(a) we give the three-dimensional picture of how the initial state $c = 0.5$ moves after each step toward the vertex state. Note that the states are no longer in the set of the generalized
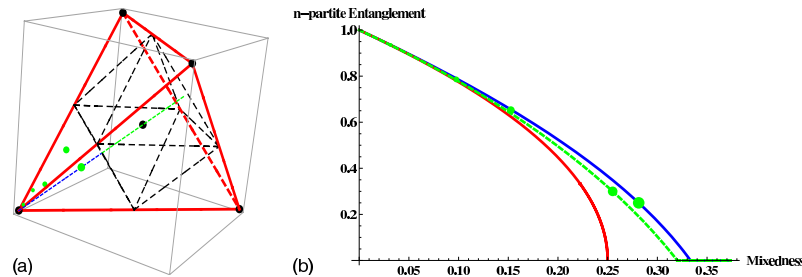
FIG. 3. (Color online) (a) Shows the final states after each step of the introduced protocol of an initial Werner or Smolin state $c=0.5$, where each (green) point represents the obtained state after one step of the protocol. (b) Shows the mixedness $[2^n/(2^n-1)][1-\mathrm{Tr}(\rho^2)]$, versus n-partite entanglement diagram (for $n=2$ the y axis has to be multiplied by 2), where the (blue) curve corresponds to the Werner or Smolin state whereas the (red) curve is the state connecting two vertices. All states of the simplex have their mixedness-entanglement ratio between these two curves. The middle (dashed, green) curve corresponds to the final states of a distilled Werner or Smolin state, and the (green) points represent the final states after each step of an initial Werner or Smolin state $c=0.5$.

Smolin sets, another advantage of the considered set of states as no random bilateral rotation to regain the rotational symmetry is needed. In Fig. 3(b) we show the mixedness-entanglement relation of this example. Note that all states of the simplex are within the two curves and the middle curve is the result for the generalized Smolin state after one step of the protocol.

Remark. Not all states of the simplex are mapped into more entangled states by this protocol. For example, the mixture of two vertex states $[\vec{c}^T=(0,0,c)$ with $c\neq 1]$ is left invariant.

In summary, we have found a protocol that increases the amount of entanglement with local operations and classical communication only and the final states are always within the class of states. Only for $n=2$ the final state is pure and maximal entangled and therefore the above protocol is a distillation protocol, i.e., pure maximally entangled states can be obtained. However, for $n>2$ the final state is no longer pure, but has the maximal n-partite entanglement of the class of states under investigation.

Thus the next logical step is to search for a distillation protocol which distills the vertex states into pure maximally entangled states, i.e., GHZ states. However, this is not possible for the following reasons. In general, any equally weighted mixture of two maximally entangled states cannot be distilled by mainly two observations. As for all maximally entangled states ρ_i obviously the entanglement can be reduced only by any completely positive map $\Lambda:\rho_i\mapsto\rho_i'$, i.e., $E(\rho_i')\leq E(\rho_i)\,\forall\,\Lambda$. And as the entanglement $E(\rho)$ is convex, i.e., $E(\rho_i')+E(\rho_j')\leq 2E(\rho_i')$, we conclude that at least one ρ_i must be mapped unitary onto itself or another maximally entangled state. Because all maximally entangled states are equivalent by local unitaries, such a map consequently maps also the other maximally entangled state of the mixture into a (different) maximally entangled state. Hence, for no equally mixture of maximally entangled states a maximally entangled state can be distilled. Note that in the case of bipartite qubits this is trivially true, because any equally mixture of Bell states is separable, however, for multipartite states this is not necessarily the case (e.g., our vertex states).

Thus we find that we can increase the amount of the n-partite entanglement until the vertex state, but not further-

more, and therefore all entangled states are bound entangled, i.e., no pure n-partite entanglement can be distilled among any subset of parties using stochastic LOCC. The common definition of distillation is that no pure maximally entanglement among any subset of parties using LOCC can be obtained; see, e.g., [23,24]. A different way to prove that the entangled states are bound is given in Ref. [25], where it is shown that if no singlets can be distilled also no GHZ state can be obtained. Therefore for the class of states under investigation we also can not distill any bipartite entanglement.

VI. THE GEOMETRY OF THE STATES VIOLATING THE CHSH-BELL INEQUALITY

Analog to the bipartite qubit state one can derive a (Clauser, Horne, Shimony, Holt) CHSH-Bell type inequality for n qubit states [26]. Here $n-1$ parties measure their qubit in the direction $\vec{a}$ or $\vec{a}$ and the nth party in the direction $\vec{b}$ or $\vec{b}$; then one obtains the following Bell inequality:

$$\mathrm{Tr}(\mathcal{B}_{\text{Bell-CHSH}}\rho)\leq 2 \qquad (27)$$

with

$$\mathcal{B}_{\text{Bell-CHSH}}=\underbrace{\vec{a}\vec{\sigma}\otimes\vec{a}\vec{\sigma}\otimes\ldots\otimes\vec{a}\vec{\sigma}}_{n-1}\otimes(\vec{b}+\vec{b}')\vec{\sigma}$$
$$+\underbrace{\vec{a}'\vec{\sigma}\otimes\vec{a}'\vec{\sigma}\otimes\ldots\otimes\vec{a}'\vec{\sigma}}_{n-1}\otimes(\vec{b}-\vec{b}')\vec{\sigma} \qquad (28)$$

where $\vec{a},\vec{a},\vec{b},\vec{b}'$ are real unit vectors and the value 2 is the upper bound on any local realistic theory.

It is known that for $n=2$ the maximal violation by quantum mechanics can simply be derived by the state ρ itself [27]. A matrix ρ violates the Bell-CHSH inequality if and only if $\mathcal{M}(\rho)\geq 1$, where $\mathcal{M}(\rho)$ is the sum of the two largest eigenvalues of the Hermitian matrix $C^\dagger C$ with $(C)_{ij}=\mathrm{Tr}(\sigma_i\otimes\sigma_j\rho)$. A generalization for n qubits is simple, because the matrix C is diagonal for the states under investigation, and thus the same proof works.
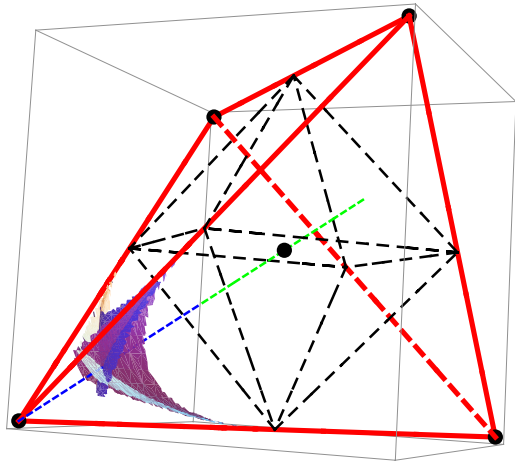
FIG. 4. (Color online) The three cylinders show the saturation of the Bell inequality. All states outside these cylinders violate the Bell inequality. The vertex states violate the Bell inequality maximally, i.e., by $2\sqrt{2}$.

In our case $\mathcal{M}(\rho)$ is simply the sum of the two largest squared vector components. In particular, if c_1 and c_2 are greater than c_3 we obtain the Bell inequality

$$c_1^2 + c_2^2 \leq 1. \tag{29}$$

This gives a simple geometric interpretation of all states violating the Bell inequality. All possible saturated Bell inequalities give three different cylinders in the picture representing the state space (see Fig. 4). All states outside of these three cylinders violate the Bell inequality.

Furthermore, this result shows that an entangled state not violating the Bell inequality (27) can be transformed via the introduced protocol into a state violating the Bell inequality, leading to the conclusion that all entangled states of the picture have nonlocal features. Moreover, in agreement with Ref. [28], the possibility to construct realistic local models or not is no criterion for being bound entangled or not.

Let us also remark that Werner states ($n=2$) violate the Bell inequality for $c > 1/\sqrt{2}$ whereas successful teleportation requires only $c > 1/2$.

VII. SUMMARY AND DISCUSSION

We generalized the magic simplex for locally maximally mixed bipartite qubit states such that we add even numbers n of qubits and set all partial traces equal to the maximally mixed states, i.e., no local information obtainable by any subset of parties is available. This class of states can be described by three real numbers, which enables us to draw a three-dimensional picture. Interestingly, we find the same geometry concerning separability, mixedness, kind of entanglement, amount of entanglement and nonlocality for all even numbers of qubits (see also Figs. 1 and 4).

For $n > 2$ the purest states, located in the vertices of the simplex, are not pure except in the case of bipartite qubits

($n=2$). We show how to derive a recently proposed measure for all discrete multipartite systems [1] in this case. For mixed states only bounds exist, however, we show that they are for the class of states optimal by proving that all states not detected by the measure are separable.

The measure reveals that these states possess only n-partite entanglement and no other kind of entanglement, e.g., bipartite entanglement. The information content of the states can be quantified by the generalized Bohr's complementarity relation for $n > 2$

$$n = \mathcal{S} + E_n + R = 1 + R, \tag{30}$$

where R is lack of classical knowledge and $\mathcal{S}=0$ the local information obtainable by any party.

Then we investigated the question whether the n-partite entanglement can be distilled. We find a protocol using only local operation and classical communication which increases the n-partite entanglement to the maximal entanglement of the class of states under investigation. These states are the vertex states of the simplex; for $n=2$ they are the Bell states and for $n > 2$ they are equal mixtures of such GHZ states which are obtained by applying only two flips, σ_x.

For bipartite qubits $n=2$ this protocol is a distillation protocol, i.e., pure maximally entangled states are obtained. For $n > 2$ the vertex states are not pure, therefore we search for a distillation protocol that leaves the class of states under investigation to obtain a pure n-partite maximally entangled state, i.e., the GHZ states. Indeed, we argue that such a protocol cannot be found; more precisely, any equal mixture of GHZ states cannot be distilled. Thus for the class of states under investigation all entangled states are bound entangled and herewith we found a simplex where all states are either separable or bound entangled.

In detail, we show how an initial state moves after each step of the protocol increasing the entanglement in the simplex (see Fig. 2). Moreover, we find that the states violating the CHSH-Bell-like inequality, which was shown to be optimal in this case, have for all even numbers of qubits the same geometry (see Fig. 4). These two results taken together mean that one can enhance the n-partite bound entanglement by using only LOCC until the Bell inequality is violated. Therefore, for all n-partite bound entangled states its (hidden) nonlocality is revealed and in agreement with Ref. [28] the possibility for a local realistic theory to be constructed is not a criterion for distillability, and likewise whether its entanglement can be increased by LOCC is also no criterion.

Our results suggest also that one can distinguish between bound states for which a certain entanglement measure cannot be increased by LOCC (in our case the vertex states) and states for which the entanglement can be increased by LOCC, which may be denoted as "quasibound" entangled states (all bound entangled states of the class except the vertex states). The introduced (distillation) protocol distills maximally entangled states within the set of states which are, however, not pure, but the purest of the set of states.

Last but not least we want to remark that a subset of the class of states has been considered in the literature, e.g., [4,6–8], the so-called Smolin states. For which it was shown that no Bell states may be distilled. The theorem in Ref. [25]

states that if and only if bipartite entanglement can be distilled then also GHZ states—in our terminology n-partite entanglement—can be distilled.

In summary, we have shown in this paper explicitly that the multipartite measure proposed by [1] detects all bound entanglement in the class of states and that the states do not possess bipartite entanglement and how the n-partite entanglement can be increased to a certain value.

These results not only help to reveal the mysteries of bound entanglement by refining the kind of entanglement, but they may also help to construct quantum communication scenarios where bound entangled states actually help to perform a certain process [29]. This is clearly important, when one has future applications in mind, e.g., a multipartite cryptography scenario.

APPENDIX A: PROOF THAT ALL STATES REPRESENTED BY THE OCTAHEDRON ARE SEPARABLE

To prove that all states represented by the octahedron are separable, we show that this is the case for the following points in the octahedron

$$\vec{c} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (A1)$$

As any convex combination of separable states have to be also separable, we have finalized the proof. We start with $n=2$ and show how this construction generalizes for $n=4,6,\dots$.

Suppose Alice prepares her qubits in the following two states:

$$\omega_{i,\pm}^A = \frac{1}{\sqrt{2}}(\mathbb{1}_2 \pm r_i^A \sigma_i), \quad (A2)$$

where r_i is a Bloch vector pointing in the i direction and is given by any number in $[-1,1]$. Bob does prepares his qubits in the very same way. If Alices chooses the positive i axis Bob does the same, and if Alice chooses the negative sign, Bob does the same, thus they share the following separable state if the preparation is done randomly with the same probability:

$$\rho_{i,+}^{AB} = \frac{1}{2}\omega_{i,+}^A \otimes \omega_{i,+}^B + \frac{1}{2}\omega_{i,-}^A \otimes \omega_{i,-}^B = \frac{1}{4}(\mathbb{1}_4 + r_i^A \cdot r_i^B \sigma_i \otimes \sigma_i). \quad (A3)$$

These states represent three vertices of the octahedron, thus the proof is finalized for $n=2$.

Explicitly, we find that for the generalized Smolin state ($c_1=c_2=c_3=c$), the following state is derivesd:

$$\rho_c = \sum_i \frac{1}{3}\rho_{i,+}^{AB} = \frac{1}{4}\left(\mathbb{1}_4 + \sum_i \frac{r_i^A \cdot r_i^B}{3}\sigma_i \otimes \sigma_i\right), \quad (A4)$$

therefore as $r_i^A \cdot r_i^B \in [-1,1]$ the generalized Smolin state is separable for $p \in [-\frac{1}{3},\frac{1}{3}]$.

For $n=4$ we remark that with the combination

$$\rho_{i,-}^{AB} = \frac{1}{2}\omega_{i,+}^A \otimes \omega_{i,-}^B + \frac{1}{2}\omega_{i,-}^A \otimes \omega_{i,+}^B = \frac{1}{4}(\mathbb{1}_4 - r_i^A \cdot r_i^B \sigma_i \otimes \sigma_i) \quad (A5)$$

one obtains the minus sign, and for the very same construction Alice, Bob, Charlie, and Daisy obtain the following separable states:

$$\rho_{i,+}^{AB} = \frac{1}{2}\rho_{i,+}^{AB} \otimes \rho_{i,+}^{CD} + \frac{1}{2}\rho_{i,-}^{AB} \otimes \rho_{i,-}^{CD}$$
$$= \frac{1}{4}(\mathbb{1}_4 + r_i^A \cdot r_i^B \cdot r_i^C \cdot r_i^D \sigma_i \otimes \sigma_i \otimes \sigma_i \otimes \sigma_i). \quad (A6)$$

As the combination $+-$, $-+$ gives again the minus sign, this proof generalizes for any even n.

APPENDIX B: ALL FOUR-FLIP OPERATORS FOR $n=4$

For convenience of the reader we list all four-flip operators in the Pauli matrix representation:

$$\mathcal{O}^1 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\},$$

$$\mathcal{O}^2 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x + \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\},$$

$$\mathcal{O}^3 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x + \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\},$$

$$\mathcal{O}^4 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\}. \quad (B1)$$

$$\mathcal{O}^5 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_y \otimes \sigma_x \otimes \sigma_y - \sigma_x \otimes \sigma_y \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x\},$$

$$\mathcal{O}^6 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_y \otimes \sigma_x \otimes \sigma_y + \sigma_x \otimes \sigma_y \otimes \sigma_y \otimes \sigma_x + \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x\},$$

$$\mathcal{O}^7 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \otimes \sigma_x \otimes \sigma_y - \sigma_x \otimes \sigma_y \\ \otimes \sigma_y \otimes \sigma_x + \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x\},$$

$$\mathcal{O}^8 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \otimes \sigma_x \otimes \sigma_y + \sigma_x \otimes \sigma_y \\ \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x\}. \tag{B2}$$

$$\mathcal{O}^9 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_y \\ \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x\},$$

$$\mathcal{O}^{10} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \\ \otimes \sigma_y \otimes \sigma_x + \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x\},$$

$$\mathcal{O}^{11} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_y \\ \otimes \sigma_y \otimes \sigma_x + \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x\},$$

$$\mathcal{O}^{12} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \\ \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x\}, \tag{B3}$$

$$\mathcal{O}^{13} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_y \\ \otimes \sigma_x \otimes \sigma_y - \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\},$$

$$\mathcal{O}^{14} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \\ \otimes \sigma_x \otimes \sigma_y + \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\},$$

$$\mathcal{O}^{15} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y - \sigma_x \otimes \sigma_y \\ \otimes \sigma_x \otimes \sigma_y + \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\},$$

$$\mathcal{O}^{16} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \\ \otimes \sigma_x \otimes \sigma_y - \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\}, \tag{B4}$$

[1] B. C. Hiesmayr and M. Huber, Phys. Rev. A **78**, 012342 (2008).

[2] R. A. Bertlmann, H. Narnhofer, and W. Thirring, Phys. Rev. A **66**, 032319 (2002).

[3] R. Horodecki and M. Horodecki, Phys. Rev. A **54**, 1838 (1996).

[4] R. Augusiak and P. Horodecki, Phys. Rev. A **73**, 012318 (2006).

[5] M. Murao and V. Vedral, Phys. Rev. Lett. **86**, 352 (2001).

[6] J. A. Smolin, Phys. Rev. A **63**, 032306 (2001).

[7] R. Augusiak and P. Horodecki, Phys. Rev. A **74**, 010305(R) (2006).

[8] S. Bandyopadhyay, I. Chattopadhyay, V. Roychowdhury, and D. Sarkar, Phys. Rev. A **71**, 062317 (2005).

[9] B. Baumgartner, B. C. Hiesmayr, and H. Narnhofer, Phys. Lett. A **372**, 2190 (2008).

[10] B. Baumgartner, B. C. Hiesmayr, and H. Narnhofer, J. Phys. A **40**, 7919 (2007).

[11] B. Baumgartner, B. C. Hiesmayr, and H. Narnhofer, Phys. Rev. A **74**, 032327 (2006).

[12] Ph. Krammer, e-print arXiv:08071830.

[13] R. A. Bertlmann and Ph. Krammer, Phys. Rev. A **78**, 014303 (2008).

[14] R. A. Bertlmann and Ph. Krammer, Phys. Rev. A **77**, 024303 (2008).

[15] R. A. Bertlmann and Ph. Krammer, e-print arXiv:0706.1743.

[16] L. Derkacz and L. Jakobczyk, e-print arXiv:0707.1575.

[17] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. e-print arXiv:quant-ph/0702225 (to be published).

[18] B. C. Hiesmayr and M. Huber, Phys. Lett. A **372**, 3608 (2008).

[19] A. Bramon, G. Garbarino, and B. C. Hiesmayr, Phys. Rev. A **69**, 022112 (2004).

[20] B. C. Hiesmayr and V. Vedral, e-print arXiv:quant-ph/0501015.

[21] S. Hill and W. K. Wootters, Phys. Rev. Lett. **78**, 5022 (1997).

[22] C. H. Bennett, G. Brassard, S. Popescu, B. Schumacher, J. Smolin, and W. K. Wootters, Phys. Rev. Lett. **76**, 722 (1996).

[23] W. Dür and J. I. Cirac, Phys. Rev. A **62**, 022302 (2000).

[24] P. W. Shor, J. A. Smolin, and A. V. Thapliyal, Phys. Rev. Lett. **90**, 107901 (2003).

[25] P. Horodecki and R. Horodecki, Quantum Inf. Comput. **1**, 45 (2001).

[26] Y.-C. Wu, P. Badziag, M. Wiesniak, and M. Zukowski, Phys. Rev. A **77**, 032105 (2008).

[27] M. Horodecki, P. Horodecki, and M. Horodecki, Phys. Lett. A **200**, 340 (1995).

[28] W. Dür, Phys. Rev. Lett. **87**, 230402 (2001).

[29] P. Horodecki, M. Horodecki, and R. Horodecki, Phys. Rev. Lett. **82**, 1056 (1999).

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Summary and outlook

It is one of the most seminal discoveries that quantum physics contradicts local realism. This characteristic can be ascribed to quantum entanglement and manifests itself through the violation of a Bell inequality. Closer considerations within recent years have raised the question of whether there is a discrepancy between entanglement and nonlocality. The clarification of this question is of great importance for our understanding of the theory, and also might have consequences for future applications. The aim of this diploma thesis was to give an overview on the latest state of knowledge in this field, and to confront entanglement with the violation of the CGLMP inequality for a certain set of states that is called the magic simplex.

We began our study in Chapter 1 with an introduction to the mathematical framework including important operator bases such as the Pauli operator basis for qubits and its generalisations for d-dimensional systems, that is the Gell-Mann and the Weyl operator basis. Afterwards, we discussed several issues concerning entanglement. We showed that it is very demanding to establish whether a mixed bipartite qudit state with $d > 2$ is separable or entangled, because of the fact that all known practical criteria (e.g. PPT and matrix realignment) are only necessary but not sufficient for separability. We reviewed the requirements for entanglement measures and presented possible candidates based on distance and convex roof. In addition, we provided the proof that entangled PPT states cannot be distilled via "local operations and classical communication".

In Chapter 2 we made clear the contradiction of quantum physics with local realistic theories. In particular, we explicitly derived that any local realistic description of a bipartite d-dimensional system obeys the CGLMP inequality, whereas quantum physics predicts a violation for the maximally entangled state. We investigated the problem of determining if a given state ρ is able to violate the CGLMP inequality and therefore non-local. This is a high-dimensional nonlinear optimisation problem where all possible measurement settings of both parties have to be taken into account. An analytical solution has been found only for the case $d = 2$. In order to study the nonlocality of higher dimensional systems, we have developed a numerical optimisation algorithm which utilises the generalised Euler angle parameterisation of $SU(N)$ and the Nelder-Mead method. The advantages of our method are its robustness against local maxima and its adaptability to other Bell inequalities. The chapter concluded with an overview of recent approaches for clarifying the possible discrepancy between nonlocality and entanglement, such as a discussion on hidden-nonlocality, tight Bell inequalities, the maximal violation of the CGLMP inequality through non-maximally entangled states and the non-local machine.

In Chapter 3 we studied the state space of bipartite qubits with the aim of finding simple representatives of locally unitarily equivalent states. We showed that all locally maximally mixed states can be represented by elements of a tetrahedron spanned by the Bell states. We discussed the difficulties with regard to finding an extension for qudits. We introduced a possible generalisation in form of the magic simplex, which is a mixture of maximally entangled two-qudit states. Afterwards we considered the problem of separability for this set of states, and showed how it can be simplified by exploiting symmetries. Considering two- and three-parameter

families of qutrit states ($d = 3$), we used these concepts to determine PPT states and to construct optimal entanglement witnesses. In order to reveal the non-local states of this families, we applied our numerical optimisation algorithm. As expected, we found that there is a large region of entangled states that do not violate the CGLMP inequality. We made a supposition about the exact form of the boundary of CGLMP violation for the three-parameter family of states on a line, which coincides with the numerical data up to the order 10^{-5}. Comparing two three-parameter families, we revealed that for the mixtures off a line, the region of nonlocality is smaller while the region of entanglement is larger. This has demonstrated that entanglement and nonlocality do not behave conformably in any case. In addition we presented a publication of our group, where we investigated a generalisation of the tetrahedron for multipartite qubit systems. Investigating separability, we realised that all entangled states in this tetrahedron are bound entangled. We showed that there is a relation between distillability and the available type of entanglement. In the multipartite case, entanglement can be shared in many different ways. In our publication we argued that bipartite Bell states cannot be distilled from the occuring entangled states, due to the fact that they only possess n-partite ($n \neq 2$) entanglement.

We conclude with some remarks regarding future research. As we have seen in this thesis, there is an abundance of open problems that make further considerations desirable. In order to solve them, progress is needed in the theory of nonlocality and entanglement. This means that Bell inequalities have to be improved, or alternatively it has to be shown that this is impossible. In addition, it is necessary to find more advanced techniques to solve the separability problem. Without developments in this field high-dimensional and/or multipartite systems are almost impossible to study. Once this has been achieved, we might be able to fully understand the relation between nonlocality and entanglement.

A MATHEMATICA notebook: Partial transposition of multipartite density matrices

```
In[1]:=  basis[dimension_] :=
           Do[basevector[n] = Transpose[{UnitVector[dimension, n]}], {n, 1, dimension}]
```

```
In[2]:=  register[dimension_, systems_] :=
           Do[enumeration[n, a_] = Floor[Mod[(a - 1) / dimension ^ (n - 1), systems]] + 1, {n, 1, systems}]
```

```
In[3]:=  registerswap[dimension_, systems_, subsystem_] :=
           Do[If[n ≠ systems + 1 - subsystem, enumerationswap[n, a_, b_] =
             Floor[Mod[(a - 1) / dimension ^ (n - 1), dimension]] + 1, enumerationswap[n, a_, b_] =
             Floor[Mod[(b - 1) / dimension ^ (n - 1), dimension]] + 1], {n, 1, systems}]
```

```
In[4]:=  TensorProducts[systems_, a_] :=
           {v = {1}; Do[v = KroneckerProduct[basevector[enumeration[n, a]], v], {n, 1, systems}]; v}
```

```
In[5]:=  TensorProductsswap[systems_, a_, b_] := {v = {1};
            Do[v = KroneckerProduct[basevector[enumerationswap[n, a, b]], v], {n, 1, systems}]; v}
```

```
In[6]:=  pt[matrix_, systems_, subsystem_] :=
           {dimension = (Dimensions[matrix][[1]]) ^ (1 / systems); basis[dimension];
             register[dimension, systems]; registerswap[dimension, systems, subsystem];
             Sum[ TensorProductsswap[systems, x1, x2][[1]].
               ConjugateTranspose[TensorProductsswap[systems, x2, x1][[1]]] * matrix[[x1, x2]],
             {x1, dimension^systems}, {x2, dimension^systems}]}[[1]]
```

```
In[7]:=  (* partialtranspose for multipartite systems of same dimension *)
```

```
In[8]:=  (* enter: pt['matrix','systems','subsystem'] *)
```

```
In[9]:=  (* matrix: self-explanatory, systems: number of systems (Integer),
           subsystem: target system for transposition (Integer) *)
```

```
In[10]:=  (*Example*)
```

$$
In[11]:= pt\left[\begin{pmatrix} 1 & 2 & 8 & 2 \\ 8 & 3 & 2 & 4 \\ 9 & 6 & 1 & 2 \\ 3 & 5 & 4 & 7 \end{pmatrix}, 2, 2\right]
$$

$$
Out[11]= \begin{pmatrix} 1 & 8 & 8 & 2 \\ 2 & 3 & 2 & 4 \\ 9 & 3 & 1 & 4 \\ 6 & 5 & 2 & 7 \end{pmatrix}
$$

B MATHEMATICA notebook: Optimisation of $\mathcal{B}_{I_3}$

In[1]:= `(* The Gell-Mann matrices are defined *)`

In[2]:= `λ2 =` $\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ `; λ3 =` $\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ `; λ5 =` $\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}$ `; λ8 = 1 / Sqrt[3]` $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$ `;`

In[3]:= `(* The generalized Euler angles for the four observables A1,A2,B1,B2 are introduced *)`

In[4]:= `ΩA1 = Array[αA1, 8]; Element[ΩA1, Reals]`

Out[4]= $(\alpha A1(1) \,|\, \alpha A1(2) \,|\, \alpha A1(3) \,|\, \alpha A1(4) \,|\, \alpha A1(5) \,|\, \alpha A1(6) \,|\, \alpha A1(7) \,|\, \alpha A1(8)) \in \mathbb{R}$

In[5]:= `ΩA2 = Array[αA2, 8]; Element[ΩA2, Reals]`

Out[5]= $(\alpha A2(1) \,|\, \alpha A2(2) \,|\, \alpha A2(3) \,|\, \alpha A2(4) \,|\, \alpha A2(5) \,|\, \alpha A2(6) \,|\, \alpha A2(7) \,|\, \alpha A2(8)) \in \mathbb{R}$

In[6]:= `ΩB1 = Array[αB1, 8]; Element[ΩB1, Reals]`

Out[6]= $(\alpha B1(1) \,|\, \alpha B1(2) \,|\, \alpha B1(3) \,|\, \alpha B1(4) \,|\, \alpha B1(5) \,|\, \alpha B1(6) \,|\, \alpha B1(7) \,|\, \alpha B1(8)) \in \mathbb{R}$

In[7]:= `ΩB2 = Array[αB2, 8]; Element[ΩB2, Reals]`

Out[7]= $(\alpha B2(1) \,|\, \alpha B2(2) \,|\, \alpha B2(3) \,|\, \alpha B2(4) \,|\, \alpha B2(5) \,|\, \alpha B2(6) \,|\, \alpha B2(7) \,|\, \alpha B2(8)) \in \mathbb{R}$

In[8]:= `AV = Flatten[{ΩA1, ΩA2, ΩB1, ΩB2}];`

In[9]:= `Do[NB[i] = {AV[[i]], 0, 2 * Pi}, {i, 1, 32}]; domain = Array[NB, 32];`

In[10]:= `(* The Euler angle parametrizations of UA1,UA2,UB1,UB2 are defined *)`

In[11]:= `UA1 := MatrixExp[i * λ3 * ΩA1[[1]]].MatrixExp[i * λ2 * ΩA1[[2]]].`
`    MatrixExp[i * λ3 * ΩA1[[3]]].MatrixExp[i * λ5 * ΩA1[[4]]].MatrixExp[i * λ3 * ΩA1[[5]]].`
`    MatrixExp[i * λ2 * ΩA1[[6]]].MatrixExp[i * λ3 * ΩA1[[7]]].MatrixExp[i * λ8 * ΩA1[[8]]]`

In[12]:= `UA2 := MatrixExp[i * λ3 * ΩA2[[1]]].MatrixExp[i * λ2 * ΩA2[[2]]].`
`    MatrixExp[i * λ3 * ΩA2[[3]]].MatrixExp[i * λ5 * ΩA2[[4]]].MatrixExp[i * λ3 * ΩA2[[5]]].`
`    MatrixExp[i * λ2 * ΩA2[[6]]].MatrixExp[i * λ3 * ΩA2[[7]]].MatrixExp[i * λ8 * ΩA2[[8]]]`

In[13]:= `UB1 := MatrixExp[i * λ3 * ΩB1[[1]]].MatrixExp[i * λ2 * ΩB1[[2]]].`
`    MatrixExp[i * λ3 * ΩB1[[3]]].MatrixExp[i * λ5 * ΩB1[[4]]].MatrixExp[i * λ3 * ΩB1[[5]]].`
`    MatrixExp[i * λ2 * ΩB1[[6]]].MatrixExp[i * λ3 * ΩB1[[7]]].MatrixExp[i * λ8 * ΩB1[[8]]]`

In[14]:= `UB2 := MatrixExp[i * λ3 * ΩB2[[1]]].MatrixExp[i * λ2 * ΩB2[[2]]].`
`    MatrixExp[i * λ3 * ΩB2[[3]]].MatrixExp[i * λ5 * ΩB2[[4]]].MatrixExp[i * λ3 * ΩB2[[5]]].`
`    MatrixExp[i * λ2 * ΩB2[[6]]].MatrixExp[i * λ3 * ΩB2[[7]]].MatrixExp[i * λ8 * ΩB2[[8]]]`

In[15]:= **(* The standard basis is chosen and the basis transformations are defined *)**

In[16]:= $v = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\};$

In[17]:= **eigA1[k_] := UA1.v[[k + 1]]**

In[18]:= **eigA2[k_] := UA2.v[[k + 1]]**

In[19]:= **eigB1[k_] := UB1.v[[k + 1]]**

In[20]:= **eigB2[k_] := UB2.v[[k + 1]]**

In[21]:= **oA1[k_] := eigA1[k].ConjugateTranspose[eigA1[k]]**
oA2[k_] := eigA2[k].ConjugateTranspose[eigA2[k]]
oB1[l_] := eigB1[l].ConjugateTranspose[eigB1[l]]
oB2[l_] := eigB2[l].ConjugateTranspose[eigB2[l]]

In[25]:= **(* The Bell inequality I3 is defined *)**

In[26]:= $\mathbf{p[rho\_, q\_, w\_, k\_] := \sum_{j=0}^{2} Tr[rho.KroneckerProduct[q[Mod[j+k, 3]], w[j]]]}$

In[27]:= **i3[state_] := (p[state, oA1, oB1, 0] + p[state, oA2, oB1, -1] +**
p[state, oA2, oB2, 0] + p[state, oA1, oB2, 0]) - (p[state, oA1, oB1, -1] +
p[state, oA2, oB1, 0] + p[state, oA2, oB2, -1] + p[state, oA1, oB2, 1])

In[28]:= **(* The maximization procedure is defined and the parameters are chosen *)**

In[29]:= **i3max[rho_] := NMaximize[Re[i3[rho]], domain, MaxIterations → 200,**
Method → {"NelderMead", "ShrinkRatio" → 0.8, "ContractRatio" → 0.8,
"ReflectRatio" → 1.6, "ExpandRatio" → 1.6, "Tolerance" → 0.1, "RandomSeed" → n}];

In[30]:= **(* The command 'compute' executes the**
maximization algorithm ten times with random simplices *)

In[31]:= **compute[rho_] := Do[max[n] = i3max[rho], {n, 10}];**

In[32]:= **(* The command 'maximum' yields the global**
maximum of I3 and the corresponding Euler angles *)

In[33]:= **maximum := Array[max, 10][[Ordering[Array[max, 10], -1]]]**

```
(* Example: Ω00 Bell state *)
```

$$\Psi = \frac{1}{\sqrt{3}} \sum_{j=0}^{2} \texttt{KroneckerProduct[v[[j+1]], v[[j+1]]];}$$

rhotest = Ψ.ConjugateTranspose[Ψ]

$$\begin{pmatrix}
\frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3}
\end{pmatrix}$$

compute[rhotest]

maximum

```
{{2.87293, {αA1[1] -> 5.72532, αA1[2] -> -0.520624, αA1[3] -> 1.21827,
    αA1[4] -> 1.71354, αA1[5] -> 6.73672, αA1[6] -> 9.07066, αA1[7] -> 1.79378,
    αA1[8] -> 1.95697, αA2[1] -> 2.95736, αA2[2] -> 3.32492, αA2[3] -> 0.0909413,
    αA2[4] -> 2.28172, αA2[5] -> 4.86642, αA2[6] -> 0.375456, αA2[7] -> 5.67429,
    αA2[8] -> 3.36199, αB1[1] -> 5.06768, αB1[2] -> 3.98113, αB1[3] -> 2.08775,
    αB1[4] -> 1.74692, αB1[5] -> 3.09829, αB1[6] -> 5.75545, αB1[7] -> 5.81317,
    αB1[8] -> 0.711775, αB2[1] -> 2.40796, αB2[2] -> 3.38539, αB2[3] -> 0.706663,
    αB2[4] -> 5.1078, αB2[5] -> 4.34756, αB2[6] -> 2.80554, αB2[7] -> 4.09544,
    αB2[8] -> 9.06912}}}
```

C   MATHEMATICA notebook: Optimisation of $\mathcal{B}_{I_4}$

In[1]:= **(* The Gell-Mann matrices are defined *)**

In[2]:= $\lambda 2 = \begin{pmatrix} 0 & -I & 0 & 0 \\ I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ **; $\lambda 3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$; $\lambda 5 = \begin{pmatrix} 0 & 0 & -I & 0 \\ 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$;**

$\lambda 8 = 1 / \text{Sqrt}[3] \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ **; $\lambda 10 = \begin{pmatrix} 0 & 0 & 0 & -I \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 \end{pmatrix}$; $\lambda 15 = 1 / \text{Sqrt}[6] \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}$;**

In[3]:= **(* The generalized Euler angles for the four observables A1,A2,B1,B2 are introduced *)**

In[4]:= **ΩA1 = Array[αA1, 15]; Element[ΩA1, Reals]**

Out[4]= $(\alpha A1(1) \,|\, \alpha A1(2) \,|\, \alpha A1(3) \,|\, \alpha A1(4) \,|\, \alpha A1(5) \,|\, \alpha A1(6) \,|$
$\alpha A1(7) \,|\, \alpha A1(8) \,|\, \alpha A1(9) \,|\, \alpha A1(10) \,|\, \alpha A1(11) \,|\, \alpha A1(12) \,|\, \alpha A1(13) \,|\, \alpha A1(14) \,|\, \alpha A1(15)) \in \mathbb{R}$

In[5]:= **ΩA2 = Array[αA2, 15]; Element[ΩA2, Reals]**

Out[5]= $(\alpha A2(1) \,|\, \alpha A2(2) \,|\, \alpha A2(3) \,|\, \alpha A2(4) \,|\, \alpha A2(5) \,|\, \alpha A2(6) \,|$
$\alpha A2(7) \,|\, \alpha A2(8) \,|\, \alpha A2(9) \,|\, \alpha A2(10) \,|\, \alpha A2(11) \,|\, \alpha A2(12) \,|\, \alpha A2(13) \,|\, \alpha A2(14) \,|\, \alpha A2(15)) \in \mathbb{R}$

In[6]:= **ΩB1 = Array[αB1, 15]; Element[ΩB1, Reals]**

Out[6]= $(\alpha B1(1) \,|\, \alpha B1(2) \,|\, \alpha B1(3) \,|\, \alpha B1(4) \,|\, \alpha B1(5) \,|\, \alpha B1(6) \,|$
$\alpha B1(7) \,|\, \alpha B1(8) \,|\, \alpha B1(9) \,|\, \alpha B1(10) \,|\, \alpha B1(11) \,|\, \alpha B1(12) \,|\, \alpha B1(13) \,|\, \alpha B1(14) \,|\, \alpha B1(15)) \in \mathbb{R}$

In[7]:= **ΩB2 = Array[αB2, 15]; Element[ΩB2, Reals]**

Out[7]= $(\alpha B2(1) \,|\, \alpha B2(2) \,|\, \alpha B2(3) \,|\, \alpha B2(4) \,|\, \alpha B2(5) \,|\, \alpha B2(6) \,|$
$\alpha B2(7) \,|\, \alpha B2(8) \,|\, \alpha B2(9) \,|\, \alpha B2(10) \,|\, \alpha B2(11) \,|\, \alpha B2(12) \,|\, \alpha B2(13) \,|\, \alpha B2(14) \,|\, \alpha B2(15)) \in \mathbb{R}$

In[8]:= **AV = Flatten[{ΩA1, ΩA2, ΩB1, ΩB2}];**

In[9]:= **Do[NB[i] = {AV[[i]], 0, 2 * Pi}, {i, 1, 60}]; domain = Array[NB, 60];**

In[10]:= **(* The Euler angle parametrizations of UA1,UA2,UB1,UB2 are defined *)**

In[11]:= **UA1 := MatrixExp[i * λ3 * ΩA1[[1]]].MatrixExp[i * λ2 * ΩA1[[2]]].MatrixExp[i * λ3 * ΩA1[[3]]].**
MatrixExp[i * λ5 * ΩA1[[4]]].MatrixExp[i * λ3 * ΩA1[[5]]].MatrixExp[i * λ10 * ΩA1[[6]]].
MatrixExp[i * λ3 * ΩA1[[7]]].MatrixExp[i * λ2 * ΩA1[[8]]].MatrixExp[i * λ3 * ΩA1[[9]]].
MatrixExp[i * λ5 * ΩA1[[10]]].MatrixExp[i * λ3 * ΩA1[[11]]].MatrixExp[i * λ2 * ΩA1[[12]]].
MatrixExp[i * λ3 * ΩA1[[13]]].MatrixExp[i * λ8 * ΩA1[[14]]].MatrixExp[i * λ15 * ΩA1[[15]]]

In[12]:= **UA2 := MatrixExp[i * λ3 * ΩA2[[1]]].MatrixExp[i * λ2 * ΩA2[[2]]].MatrixExp[i * λ3 * ΩA2[[3]]].**
MatrixExp[i * λ5 * ΩA2[[4]]].MatrixExp[i * λ3 * ΩA2[[5]]].MatrixExp[i * λ10 * ΩA2[[6]]].
MatrixExp[i * λ3 * ΩA2[[7]]].MatrixExp[i * λ2 * ΩA2[[8]]].MatrixExp[i * λ3 * ΩA2[[9]]].
MatrixExp[i * λ5 * ΩA2[[10]]].MatrixExp[i * λ3 * ΩA2[[11]]].MatrixExp[i * λ2 * ΩA2[[12]]].
MatrixExp[i * λ3 * ΩA2[[13]]].MatrixExp[i * λ8 * ΩA2[[14]]].MatrixExp[i * λ15 * ΩA2[[15]]]

In[13]:= **UB1 := MatrixExp[i * λ3 * ΩB1[[1]]].MatrixExp[i * λ2 * ΩB1[[2]]].MatrixExp[i * λ3 * ΩB1[[3]]].**
MatrixExp[i * λ5 * ΩB1[[4]]].MatrixExp[i * λ3 * ΩB1[[5]]].MatrixExp[i * λ10 * ΩB1[[6]]].
MatrixExp[i * λ3 * ΩB1[[7]]].MatrixExp[i * λ2 * ΩB1[[8]]].MatrixExp[i * λ3 * ΩB1[[9]]].
MatrixExp[i * λ5 * ΩB1[[10]]].MatrixExp[i * λ3 * ΩB1[[11]]].MatrixExp[i * λ2 * ΩB1[[12]]].
MatrixExp[i * λ3 * ΩB1[[13]]].MatrixExp[i * λ8 * ΩB1[[14]]].MatrixExp[i * λ15 * ΩB1[[15]]]

In[14]:= **UB2 := MatrixExp[i * λ3 * ΩB2[[1]]].MatrixExp[i * λ2 * ΩB2[[2]]].MatrixExp[i * λ3 * ΩB2[[3]]].**
MatrixExp[i * λ5 * ΩB2[[4]]].MatrixExp[i * λ3 * ΩB2[[5]]].MatrixExp[i * λ10 * ΩB2[[6]]].
MatrixExp[i * λ3 * ΩB2[[7]]].MatrixExp[i * λ2 * ΩB2[[8]]].MatrixExp[i * λ3 * ΩB2[[9]]].
MatrixExp[i * λ5 * ΩB2[[10]]].MatrixExp[i * λ3 * ΩB2[[11]]].MatrixExp[i * λ2 * ΩB2[[12]]].
MatrixExp[i * λ3 * ΩB2[[13]]].MatrixExp[i * λ8 * ΩB2[[14]]].MatrixExp[i * λ15 * ΩB2[[15]]]

In[15]:= **(* The standard basis is chosen and the basis transformations are defined *)**

In[16]:= $v = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\};$

In[17]:= **eigA1[k_] := UA1.v[[k + 1]]**

In[18]:= **eigA2[k_] := UA2.v[[k + 1]]**

In[19]:= **eigB1[k_] := UB1.v[[k + 1]]**

In[20]:= **eigB2[k_] := UB2.v[[k + 1]]**

In[21]:= **oA1[k_] := eigA1[k].ConjugateTranspose[eigA1[k]]**
oA2[k_] := eigA2[k].ConjugateTranspose[eigA2[k]]
oB1[l_] := eigB1[l].ConjugateTranspose[eigB1[l]]
oB2[l_] := eigB2[l].ConjugateTranspose[eigB2[l]]

In[25]:= **(* The Bell inequality I4 is defined *)**

In[26]:= $\mathbf{p[rho\_, q\_, w\_, k\_] := \sum_{j=0}^{3} Tr[rho.KroneckerProduct[q[Mod[j+k, 4]], w[j]]]}$

In[27]:= **i4[state_] :=**
Sum[(1 - 2 * k / 3) ((p[state, oA1, oB1, k] + p[state, oA2, oB1, -1 - k] + p[state, oA2, oB2, k] +
p[state, oA1, oB2, -k]) - (p[state, oA1, oB1, -1 - k] + p[state, oA2, oB1, k] +
p[state, oA2, oB2, -1 - k] + p[state, oA1, oB2, 1 + k])), {k, 0, 1}]

In[28]:= **(* The maximization procedure is defined and the parameters are chosen *)**

In[29]:= **i4max[rho_] := NMaximize[Re[i4[rho]], domain, MaxIterations → 200,**
Method → {"NelderMead", "ShrinkRatio" → 0.8, "ContractRatio" → 0.8,
"ReflectRatio" → 1.6, "ExpandRatio" → 1.6, "Tolerance" → 0.1, "RandomSeed" → n}];

In[30]:= **(* The command 'compute' executes the**
maximization procedure ten times with random simplices *)

In[31]:= **compute[rho_] := Do[max[n] = i4max[rho], {n, 10}];**

In[32]:= **(* The command 'maximum' yields the global**
maximum of I4 and the corresponding Euler angles *)

In[33]:= **maximum := Array[max, 10][[Ordering[Array[max, 10], -1]]]**

```
(* Example: Ω00 Bell state *)
```

$$\Psi = \frac{1}{2} \sum_{j=0}^{3} \text{KroneckerProduct}[v[[j+1]], v[[j+1]]];$$

```
rhotest = Ψ.ConjugateTranspose[Ψ]
```

$$\begin{pmatrix}
\frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{1}{4}
\end{pmatrix}$$

```
compute[rhotest]
```

```
maximum
```

```
{{2.89624, {αA1[1] -> 3.07265, αA1[2] -> 6.15285, αA1[3] -> 5.67497, αA1[4] -> 1.92491,
    αA1[5] -> 2.05345, αA1[6] -> 3.86138, αA1[7] -> 2.57146, αA1[8] -> 1.96996,
    αA1[9] -> 5.06114, αA1[10] -> 2.7175, αA1[11] -> 2.73205, αA1[12] -> 4.04356,
    αA1[13] -> 3.52083, αA1[14] -> 3.34487, αA1[15] -> 2.0385, αA2[1] -> 0.72059,
    αA2[2] -> 3.20978, αA2[3] -> 3.40004, αA2[4] -> 2.25048, αA2[5] -> 4.36813,
    αA2[6] -> 3.47318, αA2[7] -> 5.05212, αA2[8] -> 6.39357, αA2[9] -> 2.44141,
    αA2[10] -> 2.28185, αA2[11] -> 3.52065, αA2[12] -> 3.93748, αA2[13] -> 1.8451,
    αA2[14] -> 1.67687, αA2[15] -> 4.53126, αB1[1] -> 5.23488, αB1[2] -> 1.76584,
    αB1[3] -> 2.8723, αB1[4] -> 4.64033, αB1[5] -> 4.4815, αB1[6] -> 2.10096,
    αB1[7] -> 2.32368, αB1[8] -> 4.54152, αB1[9] -> 3.61002, αB1[10] -> 1.1092,
    αB1[11] -> 4.20415, αB1[12] -> 1.68768, αB1[13] -> 2.77742, αB1[14] -> 2.38235,
    αB1[15] -> 2.27769, αB2[1] -> 1.55276, αB2[2] -> -0.00921043, αB2[3] -> 2.56765,
    αB2[4] -> 5.51796, αB2[5] -> 3.68283, αB2[6] -> 2.72437, αB2[7] -> 4.73605,
    αB2[8] -> 4.09868, αB2[9] -> 2.13773, αB2[10] -> 2.89167, αB2[11] -> 1.43804,
    αB2[12] -> 3.99496, αB2[13] -> 1.30861, αB2[14] -> 3.90506, αB2[15] -> 2.92697}}}
```

D   Computation details on $\rho = \frac{1-\alpha-\beta}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0}$

PPT:

$$w = e^{2\pi i/3}$$

$$c_{0,0} = \frac{1-\alpha-\beta}{9} + \alpha$$

$$c_{1,0} = \frac{1-\alpha-\beta}{9} + \beta$$

$$c_{k,l} = \frac{1-\alpha-\beta}{9} \qquad \forall\,(k,l) \notin \{(0,0),(1,0)\}$$

$$(B_0)_{s,t} = \frac{1}{3}\sum_{k=0}^{2} c_{k,s+t}\,w^{k(s-t)}$$

$$\Rightarrow B_0 = \begin{pmatrix} \frac{1}{9}(2\alpha+2\beta+1) & 0 & 0 \\ 0 & \frac{1}{9}(-\alpha-\beta+1) & \frac{1}{3}\left(\alpha+\beta e^{-\frac{2\pi i}{3}}\right) \\ 0 & \frac{1}{3}\left(\alpha+\beta e^{\frac{2\pi i}{3}}\right) & \frac{1}{9}(-\alpha-\beta+1) \end{pmatrix}$$

$$\Rightarrow \det B_0 = -\frac{1}{729}(2\alpha+2\beta+1)(8\alpha^2+8\beta^2-11\alpha\beta+2\alpha+2\beta-1)$$

E   Computation details on $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{2,0}$

PPT:

$$w = e^{2\pi i/3}$$

$$c_{0,0} = \frac{1-\alpha-\beta-\gamma}{9} + \alpha$$

$$c_{1,0} = \frac{1-\alpha-\beta-\gamma}{9} + \beta$$

$$c_{2,0} = \frac{1-\alpha-\beta-\gamma}{9} + \gamma$$

$$c_{k,l} = \frac{1-\alpha-\beta-\gamma}{9} \qquad \forall\, (k,l) \notin \{(0,0),(1,0),(2,0)\}$$

$$(B_0)_{s,t} = \frac{1}{3}\sum_{k=0}^{2} c_{k,s+t} w^{k(s-t)}$$

$$\Rightarrow B_0 = \begin{pmatrix} \frac{1}{9}(2\alpha+2\beta+2\gamma+1) & 0 & 0 \\ 0 & \frac{1}{9}(-\alpha-\beta-\gamma+1) & \frac{1}{3}\left(\alpha+\beta e^{-\frac{2\pi i}{3}}+\gamma e^{\frac{2\pi i}{3}}\right) \\ 0 & \frac{1}{3}\left(\alpha+\beta e^{\frac{2\pi i}{3}}+\gamma e^{-\frac{2\pi i}{3}}\right) & \frac{1}{9}(-\alpha-\beta-\gamma+1) \end{pmatrix}$$

$$\Rightarrow \det B_0 = -\frac{1}{729}(2\alpha+2\beta+2\gamma+1)$$
$$\cdot\, (8\alpha^2 + 8\beta^2 + 8\gamma^2 + 2\alpha + 2\beta + 2\gamma - 11\beta\alpha - 11\alpha\gamma - 11\beta\gamma - 1)$$

F Computation details on $\rho = \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{0,0} + \beta P_{1,0} + \gamma P_{0,1}$

PPT:

$$w = e^{2\pi i/3}$$

$$c_{0,0} = \frac{1 - \alpha - \beta - \gamma}{9} + \alpha$$

$$c_{1,0} = \frac{1 - \alpha - \beta - \gamma}{9} + \beta$$

$$c_{0,1} = \frac{1 - \alpha - \beta - \gamma}{9} + \gamma$$

$$c_{k,l} = \frac{1 - \alpha - \beta - \gamma}{9} \qquad \forall\,(k,l) \notin \{(0,0),(1,0),(0,1)\}$$

$$(B_0)_{s,t} = \frac{1}{3}\sum_{k=0}^{2} c_{k,s+t} w^{k(s-t)}$$

$$\Rightarrow B_0 = \begin{pmatrix} \frac{1}{9}(2\alpha + 2\beta - \gamma + 1) & \frac{\gamma}{3} & 0 \\ \frac{\gamma}{3} & \frac{1}{9}(-\alpha - \beta - \gamma + 1) & \frac{1}{3}\left(\alpha + \beta e^{-\frac{2\pi i}{3}}\right) \\ 0 & \frac{1}{3}\left(\alpha + \beta e^{\frac{2\pi i}{3}}\right) & \frac{1}{9}(-\alpha - \beta + 2\gamma + 1) \end{pmatrix}$$

$$\Rightarrow \det B_0 = \frac{1}{729}(-16\alpha^3 - 16\beta^3 - 16\gamma^3 + 6\beta\alpha^2 + 6\gamma\alpha^2 + 6\gamma^2\alpha + 6\beta^2\alpha + 6\beta^2\gamma$$
$$+ 6\beta\gamma^2 - 12\alpha^2 - 12\beta^2 - 12\gamma^2 + 3\beta\alpha + 3\gamma\alpha + 3\beta\gamma - 15\beta\gamma\alpha + 1)$$

References

[1] A. Einstein, B. Podolsky and N. Rosen
Can quantum-mechanical description of physical reality be considered complete?
Phys. Rev. 47, 777 (1935)

[2] A. Aspect, J. Dalibard and G. Roger
Experimental test of Bell's inequalities using time-varying analyzers
Phys. Rev. Lett. 49, 1804 (1982)

[3] J. Audretsch
Entangled systems
Wiley-VCH (2007)

[4] J. Preskill
Lecture notes
theory.caltech.edu/people/preskill (1998)

[5] R. Horodecki, P. Horodecki, M. Horodecki and K. Horodecki
Quantum entanglement
Overview (2007) □ *arXiv: quant-ph/0702225*

[6] R. Bertlmann and P. Krammer
Bloch vectors for qudits
J. Phys. A: Math.Theor. 41, 235303 (2008) □ *arXiv: 0806.1174*

[7] M. Horodecki, P. Horodecki, and R. Horodecki
Separability of mixed states: necessary and sufficient conditions
Phys. Lett. A 223, 1 (1996) □ *arXiv: quant-ph/9605038*

[8] M. Horodecki and P. Horodecki
Reduction criterion of separability and limits for a class of distillation protocols
Phys. Rev. A 59, 4206 (1999) □ *arXiv: quant-ph/9708015*

[9] A. Peres
Separability Criterion for Density Matrices
Phys. Rev. Lett. 77, 1413 (1996)

[10] M. Horodecki, P. Horodecki and R. Horodecki
Separability of mixed quantum states: linear contractions approach
Open Syst. Inf. Dyn. 13, 103 (2006) □ *arXiv: quant-ph/0206008*

[11] O. Rudolph
Further results on the cross norm criterion for separability
Quantum Inf. Processing, Vol. 4, 219 (2005) □ *arXiv: quant-ph/0202121*

[12] K. Chen and L. Wu
A matrix realignment method for recognizing entanglement
Quantum Inf. and Computation, Vol. 3, 193 (2003) □ *arXiv: quant-ph/0205017*

[13] B. Terhal
Bell Inequalities and the Separability Criterion
Phys. Lett. A 271, 319 (2000) □ *arXiv: quant-ph/9911057*

[14] M. Lewenstein, B. Kraus, J. Cirac and P. Horodecki
Optimisation of entanglement witnesses
Phys. Rev. A 62, 052310 (2000) □ *arXiv: quant-ph/0005014*

[15] G. Vidal
Entanglement monotones
J. Mod. Opt. 47, 355 (2000) □ *arXiv: quant-ph/9807077*

[16] K. Durstberger
Geometry of entanglement and decoherence in quantum systems
Dissertation, Universität Wien (2005)

[17] M. Horodecki, P. Horodecki and R. Horodecki
Limits for entanglement measures
Phys. Rev. Lett. 84, 2014 (2000) □ *arXiv: quant-ph/9908065*

[18] M. Plenio and S. Virmani
An introduction to entanglement measures
Quant. Inf. Comp. 7, 1 (2007) □ *arXiv: quant-ph/0504163*

[19] M. Donald, M. Horodecki and O. Rudolph
The uniqueness theorem for entanglement measures
J. Math. Phys. 43, 4252 (2002) □ *arXiv: quant-ph/0105017*

[20] V. Vedral, M. Plenio, M. Rippin and P. Knight
Quantifying Entanglement
Phys. Rev. Lett. 78, 2275 (1997) □ *arXiv: quant-ph/9702027*

[21] V. Vedral and M. Plenio
Entanglement Measures and Purification Procedures
Phys. Rev. A 57, 1619 (1998) □ *arXiv: quant-ph/9707035*

[22] C. Witte and M. Trucks
A new entanglement measure induced by Hilbert-Schmidt norm
Phys. Lett. A 257, 14 (1999) □ *arXiv: quant-ph/9811027*

[23] M. Ozawa
Entanglement measures and the Hilbert-Schmidt distance
Phys. Lett. A 268, 158 (2000) □ *arXiv: quant-ph/0002036*

[24] C. Bennett, D. DiVincenzo, J. Smolin and W. Wootters
Mixed State Entanglement and Quantum Error Correction
Phys. Rev. A 54, 3824 (1996) □ *arXiv: quant-ph/9604024*

[25] L. Clarisse
Entanglement Distillation
PhD thesis, University of York (2006) □ *arXiv: quant-ph/0612072*

[26] M. Choi
Completely Positive Linear Maps on Complex matrices
Linear Algebra and Its Applications, 285 (1975)

[27] C. Bennett, G. Brassard, S. Popescu,
B. Schumacher, J. Smolin and W. Wootters
Purification of Noisy Entanglement and Faithful Teleportation

via Noisy Channels
Phys. Rev. Lett. 76, 722 (1996) □ *arXiv: quant-ph/9511027*

[28] K. Vollbrecht and M. Wolf
Efficient distillation beyond qubits
Phys. Rev. A 67, 012303 (2003) □ *arXiv: quant-ph/0208152*

[29] M. Horodecki, P. Horodecki and R. Horodecki
Mixed-state entanglement and distillation:
is there a bound entanglement in nature?
Phys. Rev. Lett. 80, 5239 (1998) □ *arXiv: quant-ph/9801069*

[30] J. Bell
On the Einstein Podolsky Rosen Paradox
Physics 1, 195 (1964)

[31] D. Bohm
Quantum Theory
Prentice-Hall, New York (1951)

[32] G. Weihs, T. Jennewein, C. Simon, H. Weinfurter and Anton Zeilinger
Violation of Bell's inequality under strict Einstein locality conditions
Phys. Rev. Lett. 81, 5039 (1998) □ *arXiv:quant-ph/9810080v1*

[33] R. Horodecki, P. Horodecki and M. Horodecki
Violating Bell inequality by mixed spin-1/2-states:
necessary and sufficient condition
Phys. Lett. A200, 340 (1995)

[34] D. Collins, N. Gisin, N. Linden, S. Massar and S. Popescu
Bell Inequalities for Arbitrarily High-Dimensional Systems
Phys. Rev. Lett. 88, 040404 (2002)

[35] T. Durt, D. Kaszlikowski and M. Zukowski
Violation of local realism with quantum systems
described by N-dimensional Hilbert spaces up to N=16
Phys. Rev. A 64, 024101 (2001)

[36] T. Tilma and E. Sudarshan
Generalized Euler Angle Parametrization for SU(N)
J. Phys. A: Math. Gen. 35, 10467 (2002) □ *arXiv: math-ph/0205016v5*

[37] T. Tilma and E. Sudarshan
Generalized Euler Angle Parameterization for U(N)
with Applications to SU(N) Coset Volume Measures
J. Geom. Phys. 52, 3, 263 (2004) □ *arXiv: math-ph/0210057v5*

[38] J. Nelder and R. Mead
A Simplex Method for Function Minimization
Computer Journal, Vol. 7, 308 (1965)

[39] L. Masanes
Tight Bell inequality for d-outcome measurements correlations
Quantum Inf. and Comp., Vol. 3, No. 4, 345 (2002) □ *arXiv: quant-ph/0210073*

[40] A. Fine
Hidden Variables, Joint Probability, and the Bell Inequalities
Phys. Rev. Lett. 48, 291 (1982)

[41] D. Avis, H. Imai, T. Ito and Y. Sasaki
Deriving Tight Bell Inequalities for 2 Parties with
Many 2-valued Observables from Facets of Cut Polytopes
(2004) □ *arXiv: quant-ph/0404014v3*

[42] P. Eberhard
Background level and counter efficiencies required for a loophole-free
Einstein-Podolsky-Rosen experiment
Phys. Rev. A 47, R747 (1993)

[43] A. Acin, T. Durt, N. Gisin and J. Latorre
Quantum non-locality in two three-level systems
Phys. Rev. A 65, 052325 (2002) □ *arXiv: quant-ph/0111143v2*

[44] N. Brunner, N. Gisin and V. Scarani
Entanglement and non-locality are different resources
New J. Phys. 7, 88 (2005) □ *arXiv: quant-ph/0412109v5*

[45] N. Cerf, N. Gisin, S. Massar and S. Popescu
Quantum entanglement can be simulated without communication
Phys. Rev. Lett. 94, 220403 (2005) □ *arXiv: quant-ph/0410027v1*

[46] N. Gisin
Bell inequalities: many questions, a few answers
Contribution to a Festschrift (2007) □ *arXiv: quant-ph/0702021v2*

[47] R. Horodecki and M. Horodecki
Information-theoretic aspects of quantum inseparability of mixed states
Phys. Rev. A 54, 1838 (1996) □ *arXiv:quant-ph/9607007v1*

[48] R. Bertlmann, H. Narnhofer and W. Thirring
A Geometric Picture of Entanglement and Bell Inequalities
Phys. Rev. A 66, 032319 (2002) □ *arXiv:quant-ph/0111116v3*

[49] B. Baumgartner, B.C. Hiesmayr and H. Narnhofer
A special simplex in the state space for entangled qudits
J. Phys. A: Math. Theor. 40, 7919 (2007) □ *arXiv: quant-ph/0610100v2*

[50] H. Narnhofer
Entanglement reflected in Wigner functions
J. Phys. A 39, 7051 (2006)

[51] B. Baumgartner, B.C. Hiesmayr and H. Narnhofer
The state space for two qutrits has a phase space structure in its core
Phys. Rev. A 74, 032327 (2006) □ *arXiv: quant-ph/0606083v1*

[52] B.C. Hiesmayr
The geometry of bipartite qutrits including bound entanglement
to be published □ *eMail: beatrix.hiesmayr@univie.ac.at*

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Phys. Rev. A 78, 042327 (2008)