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Abstract

In this thesis, quantum states of two level systems (called qubits) as well as d-level systems (called qudits), $d < \infty$, are investigated. The focus is on characterizing the property of separability and entanglement of composite systems geometrically. Since to some extend this has already been investigated for two qubit or two qudits, this work presents possible generalizations for systems comprising more particles (multipartite). It also shows analytically and numerically how these generalizations affect the prevalent separability criteria such as the Peres-Horodecki criterion, the realignment criterion, the distillation of entanglement and entanglement measures. It is shown in detail how a simplex of n-partite qubit states can be constructed in the similar manner to the bipartite qubit case and why all its elements are bound entangled states. This result is published in Physical Review A 78, 042327 (2008). Furthermore, two different constructions of an n-partite W_k-simplex are presented, which both coincide for $n = 2$ with the famous magic tetrahedron. For the special cases of the tripartite W_k-simplices (W-state simplices) special symmetries of the eligible quantum systems according to the mentioned separability criteria are revealed and certain subclasses of states can be discriminated. In addition to unveiling these symmetries via this geometrical representation of quantum states, the different cuts of such simplices also allow a precise comparison of the different criteria in a visual and easy way. These facts are therefore contributing to understand and characterize composite quantum systems as well as the associated exciting phenomenon of entanglement and its future applications, such as quantum cryptography, quantum communication or a possible quantum computer.

Die vorliegende Diplomarbeit beschäftigt sich überwiegend mit Quanten-Systemen, die zwei (auch qubit genannt) oder im allgemeinsten Fall d Freiheitsgrade (auch qudit genannt) aufweisen. Insbesondere werden die Eigenschaften zusammengesetzter Quanten-Systeme bezüglich Separabilität beziehungsweise Verschränkung auf geometrische Weise dargestellt. Beruhend auf ähnlichen, bereits bekannten Überlegungen für zwei Qubit oder zwei Qudit Systeme, werden mögliche Verallgemeinerungen dieser Ergebnisse für Vielteilchensysteme präsentiert. Des Weiteren wird das Verhalten dieser Vielteilchensysteme bezüglich der gängigsten Separabilitätskriterien, wie z.B. des Peres-Horodecki Kriteriums, des Realignment Kriteriums, der Destillation von Verschränkung und Verschränkungsmaßen, sowohl numerisch als auch analytisch betrachtet.

Es wird im Einzelnen gezeigt wie, in Anlehnung an den zwei Qubit Simplex, ein n-Teilchen Simplex bestehend aus Qubit Zuständen konstruiert werden kann und warum alle Zustände in diesem Simplex 'bound-entangled' sind. Dieses Ergebnis wurde bereits in Physical Review A 78, 042327 (2008) publiziert.

Außerdem werden zwei verschiedene Konstruktionen eines n-Teilchen W_k-Simplex vorgestellt, die beide für den $n = 2$ Fall mit dem bekannten 'Magic Tetrahedron' übereinstimmen. Für den speziellen Fall des drei Teilchen W_k-Simplex (W-Zustand Simplex) werden bestimmte Symmetrien der jeweiligen Quanten Systeme bezüglich der oben erwähnten Separabilitätskriterien aufgezeigt und dementsprechend verschiedene Subklassen von Zustände eingeführt. Zusätzlich zu diesen Symmetrien können durch diese geometrische Veranschaulichung der Zustände, d.h. durch verschiedene Schnitte dieser Simplices, die verschiedenen Kriterien präzise und leicht auf optischem Wege verglichen werden. Aus diesem Grund werden die in dieser Arbeit beschriebenen Ergebnisse dazu beitragen sowohl zusammengesetzte Quanten-Systeme als auch das damit verbundene faszinierende Phänomen der Verschränkung, welches die Grundlage für zukünftige Technologien, wie etwa Quantenkryptography, Quantenkommunikation oder möglicherweise Quantencomputer, bilden wird, besser zu verstehen.

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Part I
Introduction of the Physical Formalism

CHAPTER 1

Mathematical and Physical Basics

In this thesis the description of quantum mechanics is basically formulated by using methods of the mathematical concept of functional analysis. In order to define the base in with the theory is formulated the so called *Hilbert space* has to be introduced.

➤ **Definition:**
A Hilbert space $\mathcal{H}$ over the complex body $\mathbb{C}$ is a complex vector space equipped with a scalar product, which is defined below.

Due to the fact that this work focuses on quantum systems with countably finite degrees of freedom this general definition can be restricted to a discrete Hilbert space with a fixed dimension $d > 0$, $\mathcal{H}^d$. Furthermore the so called Dirac formalism will be used as one of the several equivalent mathematical notations for the description of quantum mechanics. In this formalism a physical state is denoted by Ψ (the notation shows the connection to the solution of the Schrödinger equation [1]), which corresponds to a so called *ket vector* $|\ \rangle$, that is an element of the introduced Hilbert space $\mathcal{H}^d$ [2]. The actual ket vector associated with Ψ is commonly written as $|\Psi\rangle$. It has to be noted that via this notation the wave function is independent of any representation, e.g. spatial or momentum [3]. As it is known from Euclidean vector spaces a minimal set of orthogonal vectors can be found, which allows to construct every element of the space by a weighted sum of its element. This set is called a basis $\mathcal{B}$ and its definition is also valid for Hilbert spaces. As an example for $\mathcal{H}^d$ serves the computational base, often denoted as the set $\{|0\rangle, |1\rangle, ..., |d-1\rangle\}$ [4].

For elements of a Hilbert space the following compositions can be defined:

➤ **Scalar Product and Norm**
The scalar or inner product is already found in the definition of the Hilbert space as a property of the space itself. It fulfills the definition of a linear functional, since it takes two elements of one Hilbert space and assigns to it a complex scalar, $S(|\Psi_1\rangle \in \mathcal{H}, |\Psi_2\rangle \in \mathcal{H}) \to \mathbb{C}$.
In the Dirac notation the scalar product is written as $\langle\Psi_1|\Psi_2\rangle = c \in \mathbb{C}$. In this case $\langle\ |$ is called a *bra* or *bra-vector* and represents the dual form of an element of the Hilbert space [5]. Whenever a basis is given the vector $|\Psi\rangle$ can be represented as $|\Psi\rangle = \sum_i c_i |b_i\rangle$, with $|b_i\rangle \in \mathcal{B}$ and $c_i \in \mathbb{C}$ and corresponds to its dual by $\langle\Psi| = \sum_i c_i^* \langle b_i|$ with $\langle b_i|$ being an element of the dual basis $\mathcal{B}^\dagger$ (for a orthonormal base the equation $\langle b_i|b_j\rangle = \delta_{ij}$ holds for its elements).

[1] The Schrödinger equation in the Dirac formalism is given by $-i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle$, independent from a special representation.
[2] The representation of a continuous wave function by a discrete vector can be made w.l.o.g. in this case by restriction to a limited volume and herewith writing Ψ as the sum of eigenfunctions of the corresponding Hamilton operator.
[3] With the later defined scalar product these special representations are given by $\Psi(\vec{x},t) = \langle\vec{x}|\Psi\rangle$ and $\Psi(\vec{p},t) = \langle\vec{p}|\Psi\rangle$, respectively.
[4] The elements written in vector form are $|0\rangle = (1,0,...,0)^T, |1\rangle = (0,1,0,...,0)^T, ..., |d-1\rangle = (0,0,0,...,1)^T$, with T being the transposition.
[5] In comparison to the continuous formulation of quantum mechanics the scalar product is given by $\int \Psi_1^* \Psi_2 dx$, whereas the dual form of the wave equation is received by complex conjugation.

Since the scalar product of a Hilbert space is constructed to fulfill the triangle as well as the parallelogram inequality, a map called *norm* of ket vector, denoted by the symbol $\| \, \|$, can be constructed by $\| |\Psi\rangle \| := \sqrt{\langle \Psi | \Psi \rangle}$. From the axiomatic approach of a norm this is, as it will turn out in the course of this chapter, not the only way to define a norm on a Hilbert space.

➤ **Kronecker Product**
The Kronecker product (also called outer or dyadic product) is defined for two elements $|\Psi_1\rangle$ and $|\Psi_2\rangle$ of the same Hilbert space $\mathcal{H}$, whereas one element is again turned into its dual form. The Kronecker product, K, combines these two elements to a map, $K(|\Psi_1\rangle, |\Psi_2\rangle) \rightarrow A$, leading other elements of the Hilbert space in the same space , $A: \ \mathcal{H} \rightarrow \mathcal{H}$.
In the Dirac notation the map A is written as $|\Psi_1\rangle \langle \Psi_2|$. Whenever a basis is given, A can be written as a $d \times d$ matrix.

➤ **Tensor Product**
Another important map is the tensor product T, taking elements of two Hilbert spaces of arbitrary dimension $\mathcal{H}_A^{d_1}$ and $\mathcal{H}_B^{d_2}$ and turning them into an element of a joint Hilbert space $\mathcal{H}$, that contains both elements: $T(|\Psi_A\rangle \in \mathcal{H}_A^{d_1}, |\Psi_B\rangle \in \mathcal{H}_B^{d_2}) \rightarrow |\Psi\rangle \in \mathcal{H}^{d_1 \cdot d_2}$.
In this work such an operation is written as $|\Psi_A\rangle \otimes |\Psi_B\rangle$ or $|\Psi_A \Psi_B\rangle$.

Operator on a Hilbert space

In quantum mechanics the term operator is a widely stretched word as it is used in many situations. In common use an operator is expressing a certain physical effect. Such an effect can have various actions as for example the time evolution of a particle or its interaction with other particles. All such effects are described by applying operators to elements of the Hilbert space by using the common vector analysis or the previously introduced maps. From the mathematical point of view an infinite number of different maps or operators, respectively, can be constructed, which means that restrictions have to be made in order to allow only those that are necessary for a complete formulation of quantum mechanics. The Dirac notation allows to define an operator O without specifying its representation by applying it on one vector $|\Psi\rangle \in \mathcal{H}^d$ and assigning it to another $|\phi\rangle \in \mathcal{H}^d$:

$$|\phi\rangle = O \ |\Psi\rangle \tag{1}$$

Another important definition is the so called *expectation value* $\langle O \rangle$ of an operator with respect to an arbitrary vector $|\Psi\rangle$, which is defined by

$$\langle O \rangle_{|\Psi\rangle} := \langle \Psi | \, O \, | \Psi \rangle \, . \tag{2}$$

When a basis $\mathcal{B}$ for a $\mathcal{H}^d$ is considered the d-dimensional identity operator $\mathbb{1}_d$ can be written as $\mathbb{1}_d = \sum_{i=0}^{d-1} |b_i\rangle \langle b_i|$, with $|b_i\rangle \in \mathcal{B}$. With inserting $\mathbb{1}_d$ and applying the scalar product with an arbitrary dual vector $|n\rangle$ equation (1) can be rewritten as

$$\underbrace{\langle n|\phi\rangle}_{c_n} = \sum_{i=0}^{d-1} \langle n|O|b_i\rangle \ \underbrace{\langle b_i|\Psi\rangle}_{d_i} = O_{ni} \ d_i. \tag{3}$$

Since this is a matrix equation, every operator, that can be represented by equation (3), can be written as $d \times d$ matrix. This allows furthermore a more precise definition of such an

operator O by determining which set of states is affected by its action. This set is called the image of O. It is usually defined as complement of kernel of the operator, $Img(O) := \overline{ker(O)}$, which is the set of states that is mapped into the zero element of the Hilbert space by this operator,

$$ker(O) := \{|\Psi\rangle \in \mathcal{H}^n | O|\Psi\rangle = 0\}. \tag{4}$$

Based on this definition, certain classes of operators can be defined by referring to their properties. The most important ones that are used in this thesis are defined in the following.

- *Linear Operator*
  An operator $L \in \mathcal{H}^d$ is said to be linear, iff $L|\lambda_1\Psi_1 + \lambda_2\Psi_2\rangle = L\lambda_1|\Psi_1\rangle + L\lambda_2|\Psi_2\rangle$, with $\lambda_i \in \mathbb{C}$ and $|\Psi_i\rangle \in \mathcal{H}^d$, holds.
- *Bounded Operator*
  An operator $B \in \mathcal{H}^d$ is called bounded iff $\frac{\|B|\Psi\rangle\|}{\||\Psi\rangle\|} < \infty \; \forall \, |\Psi\rangle \in \mathcal{H}^d$.
- *Positive Operator*
  A positive operator $P \in \mathcal{H}^d$ is given when the inequality $\langle\Psi|P|\Psi\rangle > 0$ holds for all $|\Psi\rangle \in \mathcal{H}^d$.
- *Unitary Operator*
  Unitary operators U fulfill the relation $\|U|\Psi\rangle\|^2 = \langle\Psi|U^\dagger U|\Psi\rangle = \langle\Psi|\Psi\rangle$ and are hence defined by $UU^\dagger = U^\dagger U = 1$. A unitary operator is conserving the norm of an element of a Hilbert space. One representative of a unitary operator is the time evolution $U(t, t_0)$ for a time dependent quantum state, with the additional properties $|\Psi(t)\rangle = U(t, t_0)|\Psi(t_0)\rangle$, $U(t_2, t_0) = U(t_2, t_0)U(t_1, t_0)$, with $t_2 \leq t_1 \leq t_0$.
- *Hermitian Operator*
  In order to define an hermitian operator, the *adjoint operator* has to be introduced. Whenever matrix representation O_{ij} [6] is possible the adjoint operator $O^\dagger$ can be defined via complex conjugation (*) and transposition (T) as $O^\dagger := O^{*T} = O^*_{ji}$. Otherwise the equality $\langle\phi|O\Psi\rangle = \langle O^\dagger\phi|\Psi\rangle$ can be used. For hermitian operators a special case of this equality, namely $\langle\phi|O\Psi\rangle = \langle O\phi|\Psi\rangle$, holds, i.e. O is self adjoint $O^\dagger = O$. For a finite dimensional Hilbert space, which is assumed in this work, a self adjoint operator is hermitian and vice versa. As a consequence of this property the spectrum of a hermitian operator comprises only real scalars.
  A prominent example of a hermitian operator is the Hamilton operator H, that describes not only the time evolution but also the energy of a quantum system.

Density matrix formalism

When considering the case of a quantum mechanical system given as an ensemble of wave functions Ψ_i, each with a corresponding probability p_i, the whole wave package has to be represented by a statistical map. In the Dirac formalism this map is given by the so called *density matrix* or *density operator*, usually written as ρ. It is defined as

$$\rho := \sum_{i=0}^{d-1} p_i |\Psi_i\rangle\langle\Psi_i|, \tag{5}$$

[6] $O_{ij} = \langle i|O|j\rangle$

with $p_i \geq 0$, $\sum_i p_i = 1$ and $\langle \Psi_i | \Psi_i \rangle = 1$. Whenever a basis is chosen, this density operator can be written in form of a $d \times d$ density matrix. If only one element of the Hilbert space is sufficient to describe ρ, i.e. $|\Psi_i\rangle = |\Psi\rangle$ as well as $p_i = p = 1$, ρ is said to be a *pure state* $\rho_{pure} = |\Psi\rangle \langle \Psi|$ [7], if this does not hold ρ is said to be a *mixed state*. In order to satisfy the properties of a statistical map, the following statements are valid for all density operators:

- $\langle \phi | \rho | \phi \rangle \geq 0, \forall |\phi\rangle \in \mathcal{H}^d$, i.e. ρ is positive semidefinite
- $Tr(\rho) = 1$, i.e. ρ is trace class 1

Furthermore it can be shown, by using the first property, that every density operator is self adjoint, $\rho^\dagger = \rho$. For pure states the density operator also fulfills the definition of a projector, $\rho_{pure}^2 = \rho_{pure}$ (i.e. $\rho_{pure}^2 = p\,|\Psi\rangle \underbrace{\langle \Psi | \, |\Psi\rangle}_{=1} \langle \Psi| = \rho_{pure}$). Regarding the latter property of the density matrix, a useful functional, the trace operator Tr, is used, which can serve as the scalar product in this formalism. For a d dimensional Hilbert space $\mathcal{H}^d$, with the vectors $|b_i\rangle$ being elements of a basis $\mathcal{B}$, it is defined as

$$Tr(\rho) := \sum_{k=0}^{d-1} \langle b_k | \, \rho \, |b_k\rangle = \sum_{k=0}^{d-1} \langle b_k | \sum_{i=0}^{d-1} p_i \, |\Psi_i\rangle \langle \Psi_i | \, |b_k\rangle = \underbrace{\sum_{i=0}^{d-1} p_i}_{=1} \Big\langle \Psi_i \Big| \underbrace{\sum_{k=0}^{d-1} |b_k\rangle \langle b_k|}_{=1} \Psi_i \Big\rangle = 1. \quad (6)$$

As it can be seen in this equation, the result of the trace operator Tr is independent of the chosen basis and also allows to determine the expectation value of an operator A with regards to an arbitrary state ρ by

$$\begin{aligned} \langle A \rangle_\rho = & Tr(\rho A) = \sum_k \langle b_k | \, \rho A \, |b_k\rangle = \sum_k \sum_i p_i \, \langle b_k | \, |\Psi_i\rangle \langle \Psi_i | \, A \, |b_k\rangle \\ = & \sum_i p_i \, \langle \Psi_i | \, A \underbrace{\sum_k |b_k\rangle \langle b_k|}_{=1} |\Psi_i\rangle = \sum_i p_i \, \langle \Psi_i | \, A \, |\Psi_i\rangle \, . \end{aligned} \quad (7)$$

In this case the expectation value is given by a weighted sum over the vectors of the density operator, whereas for a pure state this result coincides with equation (2). It has to be noted, that two different density matrices can lead to the same probability distribution, which means that they yield the same expectation values for the same operators and therefore to the same quantum system. The question, why the expectation values are the crucial parameters for quantum systems, leads to the postulates of quantum mechanics, which are shortly sketched in the next segment.

Postulates of Quantum Mechanics

- A quantum system can be represented by a state vector $|\Psi\rangle$ of the Hilbert space $\mathcal{H}^d$. A pure state corresponds to a set of parallel vectors, $\lambda\,|\Psi\rangle$, $\lambda \in \mathbb{C}$, whereas a normed vector $\| |\Psi\rangle \| = 1$ is usually chosen as a representative, which is unique except for a phase factor $e^{i\alpha}, \alpha \geq 0$. Via superposition state vectors can be combined to a new state vector.
  A statistical quantum state is given by a density operator (5), which is the general formulation of quantum systems comprising pure states as a special case.

[7] A pure state can also be written as a single element or a ket-vector, respectively, of the Hilbert space: $|\Psi\rangle$.

➤ A measurable value (e.g. spin, energy, angular momentum etc.), also called *observable*, corresponds to a hermitian operator by its expectation value (7). The possible expectation value and measurement result, respectively, is one of the eigenvalues of this operator $\lambda_i \in \mathbb{R}$ [8]. In the course of this measurement the state ρ is projected onto the corresponding eigenvector $|a_i\rangle$. The probability to receive the i-th eigenvalue of an hermitian operator A at a measurement $P(\delta_{A,\lambda_i})$ is given by $P(\delta_{A,\lambda_i}) = \langle \delta_{A,\lambda_i} \rangle_\rho = Tr(\rho\delta_{A,\lambda_i}) = \sum_k \langle b_k|\rho\delta_{A,\lambda_i}|b_k\rangle = \sum_k \langle b_k|\rho(\sum_j \delta_{ij}\,|a_j\rangle\,\langle a_j|)|b_k\rangle = \sum_k \langle b_k|\rho\,|a_i\rangle\,\langle a_i|\,|b_k\rangle$. W.l.o.g. the $|b_k\rangle$ can be chosen to be eigenvectors of A, $|a_k\rangle$. One obtains the probability $P(\delta_{A,\lambda_i}) = \sum_k \langle a_k|\rho\,|a_i\rangle \underbrace{\langle a_i|\,|a_k\rangle}_{\delta_{ik}} = \langle a_i|\rho|a_i\rangle$. In the special case of ρ_{pure}, $P(\delta_{A,\lambda_i}) = \langle a_i|\Psi\rangle\langle\Psi|a_i\rangle = |\langle a_i|\Psi\rangle|^2 = |c_i|^2$ holds, with the c_i´s being the coefficients of expansion in the eigenbase of the operator A. That means that the squared absolute value of these coefficients denotes the probability of receiving the i-th eigenvalue of A as an observable.

In the following definition a more general mathematical way is briefly introduced, as it allows a description of quantum states and effects by special maps instead of operators. As this theory is often not only a useful alternative but also an assumedly generalization of existing results, it will be introduced and also referred to it in the further chapters.

➤ **Completely Positive Map**

In order to receive the most general definition of a completely positive (cp) map, the term of a *channel* has to be established. Following the work of [1], a channel can be seen as link between two systems, in this work two quantum systems. The first system, also called input system, is characterized by a certain algebra of its observables $\mathcal{A}$, whereas the second, the output system, in analogy by an algebra $\mathcal{B}$. The two systems are hence denoted by the set of all bounded operators over its eligible Hilbert space, $\mathcal{B}(\mathcal{H}_1)$ and $\mathcal{B}(\mathcal{H}_2)$. It will turn out that this choice of a channel connecting these two sets allows an alternative way of describing the action of operators, e.g. for the measurement process the output channel $\mathcal{B}(\mathcal{H}_2)$ would be the set of all linear functionals with the appropriate measurement outcomes.

In order to describe such a channel in a mathematical way, a single operator $B \in \mathcal{B}(\mathcal{H}_2)$ with a certain effect ϵ on quantum systems of the output system is considered. By introducing a map T, that, in the most general case, is mapping such effects of an operator of the output system to an operator of the input system,

$$T : \epsilon(\mathcal{B}(\mathcal{H}_1)) \to \epsilon(\mathcal{B}(\mathcal{H}_2)), \tag{8}$$

the link that a channel should provide is completely described [9]. When the properties and the effects of linear operators on quantum states are considered, certain propositions to T can be established in order to gain an equivalent description. For all operators (here denoted by A) T has to be linear, positive (i.e. $T(A) \geq 0, \forall A \geq 0$), bounded from above by $\mathbb{1}$ (i.e. $T(\mathbb{A}) \leq \mathbb{1}$) and trace preserving (i.e. $Tr(T(A)) = Tr(A)$). Since for describing composed quantum systems the positivity alone is no longer a sufficient criteria, the important class completely positive (cp) maps are needed.

[8] As the Hilbert space is assumed to be discrete this property also holds for the spectrum of a hermitian operator on this space.

[9] This argument also holds when instead of the set of the operators the states of the Hilbert space itself would have been introduced as input and output systems. This choice would have lead to a different map T^*, that corresponds to T as the different but equivalent description of quantum mechanics by the Heisenberg and Schrödinger picture.

Definition (completely positive map):
When two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with their corresponding observable algebras $\mathcal{A}$ and $\mathcal{B}$ are given a linear map $T : B(\mathcal{H}_A) \to B(\mathcal{H}_B)$ leading from the set of bounded operators of the Hilbert space $\mathcal{H}_A$ to the set of bounded operators of the Hilbert space $\mathcal{H}_B$ is called a completely positive map if

$$T \otimes \mathbb{1} : \mathcal{A} \otimes \mathcal{B}(\mathbb{C}^d) \to \mathcal{B} \otimes \mathcal{B}(\mathbb{C}^d) \tag{9}$$

is positive for all $d \in \mathbb{N}$.

➤ **Kraus Decomposition**

It can further be shown [2] that a cp maps $T : B(\mathcal{H}_A) \to B(\mathcal{H}_B)$ can always be written in the form

$$T(A) = \sum_{j=1}^{d} V_j^* A V_j, \tag{10}$$

whereas $d \leq dim(\mathcal{H}_A)\dot{dim}(\mathcal{H}_B)$ and $V_j : \mathcal{H}_A \to \mathcal{H}_B$. This form of a cp map is called the *Kraus decomposition* with the associated Kraus operators V_j, that fulfill the relation $\sum_j V_j^* V_j \leq 1$.
This is a corollary of the so called *Stinespring dilation theorem* [3], which claims the unique description of a positive map (up to unitary equivalence) with operators by enlarging the given Hilbert space by an ancilla. This theorem is useful as it does not only allow a direct relation between linear maps T and operators leading from one Hilbert space to another but also shows how such a map can be constructed by given operators or vice versa. There exist also other versions of this corollary, where for example the restriction to cp and trace preserving maps is demanded and leads therefore to more restrictions of the Kraus operators.

CHAPTER 2

Separable and Entangled States

2.1 Bipartite Entanglement

In this section a two particle quantum system is investigated, that is composed by elements of two Hilbert spaces, conventionally called $\mathcal{H}_{\mathrm{A(lice)}}$ and $\mathcal{H}_{\mathrm{B(ob)}}$, each with arbitrary dimensions, i.e. arbitrary degree of freedoms (d_A and d_B). A state ρ_{AB} on the composed Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_{\mathrm{Alice}} \otimes \mathcal{H}_{\mathrm{Bob}}$ is called bipartite, and defined on the $d = d_A \cdot d_B$ dimensional space $\mathcal{H}_{AB}$ as

$$\underbrace{\rho_{AB}}_{\in \mathcal{H}_{\mathrm{Alice}} \otimes \mathcal{H}_{\mathrm{Bob}}} = \sum_{i=0}^{d_A-1} \sum_{j=0}^{d_B-1} p_{ij} \underbrace{\rho_A^i}_{\in \mathcal{H}_{\mathrm{Alice}}} \otimes \underbrace{\rho_B^j}_{\in \mathcal{H}_{\mathrm{Bob}}}, \text{ with } p_{ij} \geq 0. \tag{11}$$

Furthermore the state ρ_{AB} has to fulfill the properties of a density operator, as discussed in the previous chapter.
All bipartite states can be classified into two types by restricting this definition. A bipartite state $\rho_{AB} \in \mathcal{H}_{AB}$ can either be *separable*, iff it can be written as

$$\rho_{AB,separable} = \sum_i p_i \ |a_i\rangle \langle a_i| \otimes |b_i\rangle \langle b_i| \,, \text{ with } 0 \leq p_i \leq 1 \text{ and } \sum_i p_i = 1, \tag{12}$$

and $|a_i\rangle_A$ and $|b_i\rangle_B$ being the eligible bases on $\mathcal{H}_{\mathrm{Alice}}$ and $\mathcal{H}_{\mathrm{Bob}}$, respectively. An alternative definition of separable states (with finite dimension) can be stated by using pure states [4],

$$\rho_{AB,separable} = \sum_i p_i \ \rho^i_{pure,A} \otimes \rho^i_{pure,B}, \text{ again with } 0 \leq p_i \leq 1 \text{ and } \sum_i p_i = 1. \tag{13}$$

If such a factorization is not possible the state is not separable (also called *entangled*).
For the special case of ρ_{AB} being a pure state (usually written as $|\Psi\rangle_{AB}$) equation (11) reduces to

$$|\Psi\rangle_{AB} := \rho_{AB,pure} = \sum_{ij} c_{ij} \, |a_i\rangle_A \otimes |b_j\rangle_B = \sum_{ij} c_{ij} \, |a_i b_j\rangle \,, \quad \text{with} \sum c_{ij}^2 = 1. \tag{14}$$

A pure bipartite state is separable if it can written as

$$\rho_{AB,pure,separable} = |\Psi\rangle_{AB} = |\Psi\rangle_A \otimes |\Psi\rangle_B \,. \tag{15}$$

In equation (14) this is fulfilled iff the matrix $C = \{c_{ij}\}$ has rank 1. A state, that can not be written in this form, is called a non-separable (or entangled) pure state.
This mathematical definition of entanglement suggests that an entangled state is a bipartite quantum system that can not be factorized. This phenomena leads to a fundamental difference of quantum systems compared to classical ones, as a special physical connection between such particles is found. This leads to the fact that operations performed on one particle have different results for separable and entangled state, which leads to the so called *quantum correlation* between two or more systems [10]. Along with this definition for composite quantum

[10] This correlation is discussed further in the LOCC section on page 14.

systems some helpful definitions and basic results are needed and therefore presented in the following:

➤ **Schmidt Decomposition**

The Schmidt decomposition, e.g. found in [5, 6], combines a mathematical theorem with this definition of a d-dimensional bipartite state ρ_{AB}, since it claims that a basis transformation from two individual bases of $\mathcal{H}_\mathcal{A}$ and $\mathcal{H}_\mathcal{B}$ to a certain basis in the composite Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ is always possible in such a way that the coefficients c_{ij} or p_{ij}, respectively, reduce to c_i or p_i. Due to singular value decomposition this basis transformation is unique and always possible. Before the general result of this Schmidt decomposition for arbitrary bipartite states can be posed, the definition of the *Schmidt rank* r of a pure bipartite state has to be defined [7, 8]. Hence a pure bipartite state, as defined in (14), can be rewritten in terms of a new basis $|u_i\rangle_A \in \mathcal{H}_A$, $|v_j\rangle_B \in \mathcal{H}_B$ as

$$|\Psi\rangle_{AB} = \sum_{i=0}^{r-1} c_i \, |u_i\rangle_A \otimes |v_i\rangle_B \,, \tag{16}$$

with $r \leq min(d_A, d_B)$, $c_i > 0$ and $\sum_{i=0}^{r-1} c_i^2 = 1$. The c_i are called *Schmidt coefficients*. A bipartite pure state is separable iff only one Schmidt coefficient exists that is non zero (this property leads back to the definition of separability for pure states (15)). If more than one Schmidt coefficients exist that are non zero, the state is entangled, whereas in addition all these coefficients are equal, the state is said to be *maximally entangled*. These statements only hold for the special case of bipartite pure states.
For arbitrary states this generalization of the Schmidt decomposition is valid:
A bipartite state ρ_{AB} can be decomposed in a (weighted) sum of pure states on the composed Hilbert space, each with its corresponding Schmidt rank r_i, $|\Psi_i^{r_i}\rangle \in \mathcal{H}_{AB}$. It has to be noted that this decomposition is not unique.

$$\rho_{AB} = \sum_{i=0}^{d_A-1} \sum_{j=0}^{d_B-1} p_{ij} \; \rho^i_{A,pure} \otimes \rho^j_{B,pure} \quad \longrightarrow \quad \rho_{AB} = \sum_i p_i \; |\Psi_i^{r_i}\rangle \langle \Psi_i^{r_i}| \,. \tag{17}$$

The *Schmidt number* k of a state ρ_{AB} is defined as $k = \{\min r_{\max}\}$, with $r_{\max}$ being the largest Schmidt rank of a pure state within one decomposition and k being the minimum over all maximal Schmidt ranks, $r_{\max}$, of each possible decomposition.

➤ **Maximally Entangled States**

There are several criteria that can determine the amount of entanglement of a state, i.e., from a heuristic point of view, how strong the connection between the entangled particles is. One of them is the Schmidt decomposition, that can, as stated above, define a maximally entangled pure state or another one would be the von Neumann entropy [11]. However, as it is shown in [9], every maximally entangled bipartite state, whose subsystems have equal dimension $d = d_A = d_B$, is local unitary equivalent [12] to $|\Psi^+\rangle = \frac{1}{\sqrt{d}} \sum_i^d |i, i\rangle$. This leads to the fact that the reduced density matrices of a maximally entangled state $\rho_{A/B} = Tr_{A/B} \, |\Psi^+\rangle \langle \Psi^+|$ [13] are totally mixed (i.e. $\rho_{A/B} = \mathbb{1}_d$). The bipartite qubit case serves as a basic example, i.e. two Hilbert spaces with two

[11] The von Neumann entropy S of a state ρ is defined as $S(\rho) = -Tr(\rho \log_2 \rho)$.
[12] Local unitary equivalent states can be transformed into each other by applying unitary operators on its eligible subsystems $\mathcal{H}_A$ and $\mathcal{H}_B$.
[13] $Tr_{A/B}$ denotes the trace operator applied on one of the two subsystems.

degrees of freedom, $\mathcal{H}_A^2 \otimes \mathcal{H}_B^2$ [14]. In this four dimensional space the four so called pure *Bell states* not only denote the maximally entangled states but are also a complete orthonormal set, the so called *Bell-base*.

$$\left|\Phi^{\pm}\right\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \quad \left|\Psi^{\pm}\right\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle) \tag{18}$$

➤ **LOCC Operations**

For bipartite (as well as later for multi particle systems) an important class of operations has to be introduced in order to address each particle (local subsystem) and clarify what information exchange between these subsystems is allowed [15]. One approach to characterize these operators is to determine the correlation of a multipartite quantum state. As these arguments are easily expandable to higher dimensions, a bipartite system, comprising $\mathcal{H}_A$ and $\mathcal{H}_B$, serves to understand the class of LOCC operators. Following the work of reference [10], two consecutive measurements are considered, one performed by Alice on the first subsystem and one by Bob on the second. The results of these measurement are obviously depending on whether the two subsystems are somehow connected or the quantum systems are independent from each other. Therefore if a composite quantum system can not be separated into two independent subsystems, $\rho_{AB} \neq \rho_A \otimes \rho_B$, the state is entangled (equations (12) and (13)) and hence the measurement results of the two subsystems are not independent from each other, i.e. they are correlated. This means that a separable state can either be classically correlated or not correlated, whereas an entangled state is neither. However does an entangled quantum system posses a special correlation that can not be described via classical correlation. Entangled states are therefore said to be *quantum correlated* states, which allows an information exchange that is completely unknown from a classical point of view. In order to separate these two kinds of correlations from each other, a special set of operators is defined, comprising only operators that can not create or manipulate (increase or decrease) the entanglement between the two subsystems and hence the quantum correlation. This set is called *LOCC*, standing for Local Operation and Classical Communication. Elements of this set can be for example unitary operations as well as the measurement operator, as long as it restricted to only one subsystem. This implies that Alice and Bob are allowed to prepare a quantum state on their subsystem by using LOCC operation. They can also correlate their prepared states ρ_A^i and ρ_B^i, respectively, by using classical communication and create a state ρ_{AB} ($\neq \sum_i p_i \rho_A^i \otimes \rho_B^i$) that is, due to its preparation, *classical correlated*.

For the equivalent formalism of channels introduced in chapter 1, a similar result in terms of a set of LOCC channels can be stated that preserves the classical correlation of a state. For a more detailed review it is referred to reference [1].

➤ **Operator Basis**

In analogy to a basis given by orthogonal vectors or pure states, respectively, a minimal set of operators, a so called *operator basis*, can be constructed, that allows to express every density operator of the Hilbert space as a (weighted) sum of its elements. However it has to be noted that the properties of this operator basis depend on the degree of

[14] The two adjustments of a qubit are denoted by two ket vectors, w.l.o.g. in this work by $|0\rangle$ and $|1\rangle$.
[15] For a more detailed definition of information via the Shannon-Entropy it is referred to [10].

freedom of the quantum system and the particles, respectively. For the qubit case, the elements of the operator basis are given by the three *Pauli matrices* σ_x, σ_y, σ_z (with the relations $\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$) and the identity operator $\mathbb{1}_2$.

$$\mathcal{P} = \{ \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\sigma_x}, \quad \underbrace{\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{\sigma_y}, \quad \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\sigma_z}, \quad \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{\mathbb{1}} \}. \tag{19}$$

All these matrices are elements of the $SU(2)$ group and since all their eigenvalues are either 1 or -1 also hermitian [16]. The basis itself is called the *Pauli base* $\mathcal{P}$. With this operator basis all density operators can be written as

$$\rho = \sum_{i,j=0}^{3} c_{ij}\ \sigma_i \otimes \sigma_i, \text{ with } Tr(\rho) = 1, \tag{20}$$

whereas the convenient notation $\sigma_0 = \mathbb{1}_2$, $\sigma_1 = \sigma_x$, $\sigma_2 = \sigma_y$ and $\sigma_3 = \sigma_z$ is used. The peculiarity of $\mathcal{P}$ is that all matrices are not only unitary but also hermitian, a property that can only be realized for the qubit case.
Though for quantum systems with more than two degrees of freedom, i.e. in general d (also called *qudits*), such an operator basis can be found, either the unitarity or the property of the elements being hermitian vanishes. For the qudit case with $d > 2$, two special classes of bases are known: The first one comprises unitary matrices, whereas the second possibility consists of hermitian operators. The unitary choice are called Weyl operators $W_{k,l}$, which are defined by

$$W_{k,l} := \sum_{i=0}^{d} \omega^{ik} \left|i\right\rangle \left\langle i+l\right|, \tag{21}$$

with $|i\rangle$ being an element of an orthonormal base of $\mathcal{H}^d$, $\omega = e^{\frac{2\pi i}{d}}$ and $k, l \in \{0, 1, ...d-1\}$ modulo d. Alternatively $W_{k,l}$ can be defined by their action on a pure d-dimensional state $|s\rangle$

$$W_{k,l} \left|s\right\rangle := \omega^{k(s-l)} \left|s-l\right\rangle. \tag{22}$$

One sees that there exist exactly d unitary, traceless (except for $\mathbb{1}_d$) Weyl operators. These definitions can be found in references [11, 12]
The hermitian choice would be the Gell-mann matrices. These are traceless and the infinitesimal generators of the three dimensional special unitary group $SU(3)$. As they are defined by obeying $[T^i, T^j] = if^{ijk}T^k$ with f^{ijk} being either 1, $\frac{1}{2}$ or $\frac{\sqrt{3}}{2}$, depending on the particular index combination. Possible matrix representations of the Gell-mann matrices can be taking from various sources.

2.2 Multipartite Entanglement

Before introducing the best known methods in classifying separability and entanglement, this section is dealing with possible generalizations of the previously stated definition of bipartite separability. Unlike a two particles state, whose separability can only be characterized by regarding two subsystems, the more general n particle case needs to be established with

[16] σ_x,σ_y,σ_z are not only elements but also the generators of the $SU(2)$ group.

respect to its type of separability concerning its n subsystems. Therefore a further reaching definition of separability for multipartite quantum systems has to be introduced, as it is done for instance in references [5, 6]. This more general separability is called *k-separability*

Multipartite Entanglement of pure state:
An n particle pure state $|\Psi\rangle \in \mathcal{H}_{A_1,\ldots,A_n}$ with arbitrary degrees of freedom for each one of the n subsystems A_i is called k-separable iff there exist $m-1$ "cuts " . Such a cut exists if k subsystems can be divided into two partitions each comprising $\frac{k}{2}$ subsystems (for k being even) or $\frac{k+1}{2}$ and $k-\frac{k+1}{2}$ subsystems, respectively (for k being odd). This division is possible if these two partitions are separable (equations (14),(15)). For the special case of an n-partite state with $n-1$ possible cuts, all n subsystems are mutually separable. This classifies the state to a so called *fully n-separable* state, $\left|\Psi^{fs}\right\rangle$. If on the other hand no cut is possible, no separability can be found between any of the subsystems. Hence such a state is called *genuine n-partite entangled*, $|\Psi^{ge}\rangle$. Naturally the k-separability is consistent with the previous definition of bipartite separability, since a bipartite state consists of exactly one cut that denotes the separability of two partitions, in the following denoted as $\left|\Psi^{bs}\right\rangle$. However it has to be noted that an n partite quantum state is always said to be entangled except for the special case of $n=m$, i.e. $n-1$ cuts [17]. Contrary to the $k=0$ and $k=n$ case, the partition of the bipartite separability is not unique. All these states are usually summarized by the term *partially separable*, which will be examined further afterwards. These rather abstract definitions become clearer when considering the four qubit case as an example:
A fully 4-separable qubit state is defined as

$$\left|\Psi^{fs}\right\rangle_{A_1|A_2|A_3|A_4} = |\Psi_a\rangle_{A_1} \otimes |\Psi_b\rangle_{A_2} \otimes |\Psi_c\rangle_{A_3} \otimes |\Psi_d\rangle_{A_4}\,, \tag{23}$$

with the three $(4-1)$ cuts $A_1|A_2|A_3|A_4$ denoted as the bars between the subsystems A_i. The genuine four partite entangled states, which can maybe seen as the opposite of this fs-state, would be written as

$$|\Psi^{ge}\rangle_{A_1A_2A_3A_4} = |\Psi_{abcd}\rangle_{A_1A_2A_3A_4}\,. \tag{24}$$

Beside these unique cases for $\left|\Psi^{fs}\right\rangle$ and $|\Psi^{ge}\rangle$, ten possible states are eligible for the biseparability of a 4-partite state, since there exist $\binom{4}{1}$ possible combination for the $A_i|A_jA_kA_l$ and $\binom{4}{2}$ for the $A_iA_j|A_kA_l$ case:

$$\begin{aligned}
\left|\Psi^{bs}\right\rangle_{A_1|A_2A_3A_4} &= |\Psi_a\rangle_{A_1} \otimes |\Psi_{bcd}\rangle_{A_2A_3A_4} \\
\left|\Psi^{bs}\right\rangle_{A_1A_2|A_3A_4} &= |\Psi_{ab}\rangle_{A_1A_2} \otimes |\Psi_{cd}\rangle_{A_3A_4} \\
\left|\Psi^{bs}\right\rangle_{A_1A_3|A_2A_4} &= |\Psi_{ac}\rangle_{A_1A_3} \otimes |\Psi_{bd}\rangle_{A_2A_4} \\
&\vdots
\end{aligned} \tag{25}$$

For triseparability only $\binom{4}{2}$ possible states are available, since only the $A_i|A_j|A_kA_l$ case has

[17] This means that the state can be written as a product state with n 'factors'

to be considered:

$$\begin{aligned} \left|\Psi^{ts}\right\rangle_{A_1|A_2|A_3A_4} &= \left|\Psi_a\right\rangle_{A_1} \otimes \left|\Psi_b\right\rangle_{A_2} \otimes \left|\Psi_{cd}\right\rangle_{A_3A_4} \\ \left|\Psi^{ts}\right\rangle_{A_1A_2|A_3|A_4} &= \left|\Psi_{ab}\right\rangle_{A_1A_2} \otimes \left|\Psi_c\right\rangle_{A_3} \otimes \left|\Psi_d\right\rangle_{A_4} \\ \left|\Psi^{ts}\right\rangle_{A_1A_2|A_3|A_4} &= \left|\Psi_{ac}\right\rangle_{A_1A_4} \otimes \left|\Psi_b\right\rangle_{A_2} \otimes \left|\Psi_c\right\rangle_{A_3} \\ &\vdots \end{aligned} \tag{26}$$

The description of k-separability by using cuts is a quite heuristic way. A more exact definition of this property not only for the special case of pure states but for arbitrary quantum states can be found in reference [13].

Multipartite Entanglement for arbitrary states:
The special case of a state being called fully separable is given iff it can be written as

$$\rho^{fs} := \sum_i p_i \left|\Psi_i^{fs}\right\rangle \left\langle\Psi_i^{fs}\right|. \tag{27}$$

A state $\rho \in \mathcal{H}_{A_1,...,A_n}$ with the corresponding index set $I = \{1, 2, ..., n\}$ is partial k-separable with respect to a certain partition $P_k = \{I_1, I_2, ..., I_k\}$, with I_i, I_j being a disjoint subset of I, iff

$$\rho^{\text{k-sep}} = \sum_{i=1}^{n} p_i \ \rho_1^i \otimes \rho_2^i \otimes ... \otimes \rho_k^i \tag{28}$$

with ρ_l^i being pure density operators defined on the Hilbert space, which is assigned to the index I_l. E.g. $I_1 = \{i, j, k\} \Rightarrow \rho_1 \in \mathcal{H}_{A_i} \otimes \mathcal{H}_{A_j} \otimes \mathcal{H}_{A_k}$, with $i < j < k \in I$.
If an n partite state can not be written according to this definition of a k-separable state, it is called genuine n-partite entangled.

As multipartite entanglement and separability, respectively, of n partite systems differ from the bipartite case in so many way, the characterization of the set of separable states (SEP) is still a hard task, whereas a few of the most successful steps are presented in the following chapters. One of these steps, namely the geometrical visualization of certain sets of states (simplices), will be focused in chapter 9.
After introducing the mainly used states of this work in the next chapter, the following sections will give a glimpse of the most common methods that are used to describe, discriminate, manipulate and characterize quantum states. As one will see, all of these methods were primarily developed for the bipartite case, but often generalization to n partite states can be found.

2.3 Special Multipartite States

As this work focuses on qubits, the problem of generalizing the four maximally entangled Bell states (18) for more than two qubits has to be tackled. When speaking of maximally entangled qubit states of higher dimensions one has to reconsider that there exists no approved measure. Therefore the property of a state being maximally entangled can not be answered impartial, which means further that more possible generalizations of so called *total entangled* states coexist. It is obvious that these totally entangled state are all genuine multipartite entangled in terms of equation (24). When speaking of maximally or totally entangled states of a $n \geq 2$ particle qubit systems, the eligible states are of this form:

I GHZ state

The *GHZ state*, named after Greenberger, Horn and Zeilinger, of an n particle qubit system is defined as

$$|GHZ\rangle := \frac{1}{\sqrt{2}}(\underbrace{|0\rangle \otimes |0\rangle \otimes ... \otimes |0\rangle}_{n} + \underbrace{|1\rangle \otimes |1\rangle \otimes ... \otimes |1\rangle}_{n}) := \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n}). \quad (29)$$

It is constructed via the superposition of two orthogonal states containing n subsystems, that are all in the same state $|0\rangle$ or $|1\rangle$. Due to its construction, every measurement on one subsystem reduces the GHZ state to a separable $n-1$ dimensional state. The same is also valid whenever only a certain subset of the n subsystems is investigated and others are ignored, which is mathematically expressed by the so called *partial trace* operation [18]. The entanglement property of this state can therefore only be found when all n-particles are investigated.

This special property is visualized in Figure 1 for a three particle state, with one dot representing one qubit, a continuous line the entanglement between two qubits and the dashed line the vanishing entanglement by "removing" one of the qubits.
In chapter 9 it is shown that these states can be used in order to construct certain simplices by taking convex combinations of this state and its variations. The visualization of such simplices is shown in part III of this work.

Figure 1: Entanglement of the GHZ state

II W_k states

Another possible generalization to higher dimensions is this set of states:

$$|W_k\rangle := \binom{n}{k}^{-\frac{1}{2}} (|\underbrace{11...1}_{k}\underbrace{00...0}_{n-k}\rangle + \text{Permutations}) \qquad 1 \leq k \leq \frac{n}{2} \quad (30)$$

These kind of states are called W_k *states*. They are build by the sum of $\binom{n}{k}$ terms in such a way that every possible permutation of the term, which is composed by n subsystems, whereas k subsystems are in the "1" and the remaining $n-k$ subsystems are in the "0" state, is part of this sum. Whenever one subsystem of a W_k state is ignored or measured, the remaining state may still be entangled (depending on the "direction "of the measurement, $|0\rangle$ or $|1\rangle$). This is a fundamental different behavior of entanglement compared to a GHZ state. This property becomes more obvious when investigating certain special cases of these W_k states as it is done in the following.

[18] The partial trace for a bipartite state $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$ of the first subsystem is given by $Tr_A(\rho) = \sum_k \sum_{ij} p_{ij} \langle k| |j\rangle \langle j| |k\rangle_A |j\rangle \langle j|_B = \rho_B$, with $\rho_B \in \mathcal{H}_B$ being the so called *reduced density operator*. The generalization to n dimensional states is obvious, since $Tr_{A_i,A_j,...,A_k}(\rho) : \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes ... \mathcal{H}_{A_n} \to \cdots \otimes \mathcal{H}_{A_{i-1}} \otimes \mathcal{H}_{A_{i+1}} \otimes \ldots \mathcal{H}_{A_{j-1}} \otimes \mathcal{H}_{A_{j+1}} \otimes \ldots \mathcal{H}_{A_{k-1}} \otimes \mathcal{H}_{A_{k+1}} \otimes \ldots$, with $i, j, k \in \{1, 2, ..., n\}$.

➤ **W-states**

W-states are the restriction of the W_k states for the value $k = 1$ and are for the n dimensional qubit case defined as

$$|W\rangle := \frac{1}{\sqrt{n}}(|\underbrace{100...0}_{n}\rangle + |010...0\rangle + ... + |00...1\rangle). \tag{31}$$

They describe the superposition of n particle states comprising n subsystem, whereas in every term of the sum a different subsystem is in an excited state. Due to this construction the resulting entanglement can be found in between every pair of the n particles. Considering for example the special case of a tripartite W state and the projection onto the $|0\rangle$ state on one of its subsystems. The resulting two particle state is in the maximally entangled $|\Psi\rangle^+ = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ state, contrary to the tripartite GHZ state (as well as the n-partite GHZ states), which would be a separable state after such a measurement. The similar is true for ignoring one subsystem, since the partial trace leads to the mixed entangled state $\frac{1}{3}(|00\rangle\langle 00| + |10\rangle\langle 01| + |01\rangle\langle 01|)$. In a similar way to the latter picture this property is visualized in Figure 2, whereas here the continuous drawn ellipses are representing the entanglement of two qubits

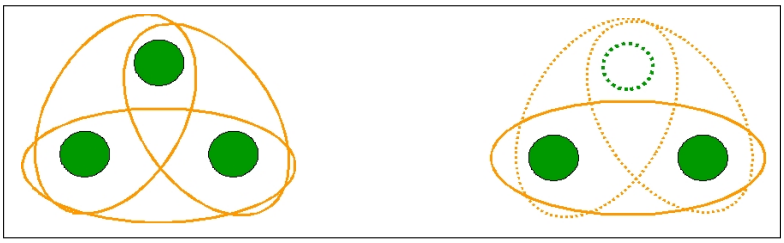


Figure 2: Entanglement of the W state

Also for these states a simplex of its Hilbert space can be constructed and visualized by special cuts of it in an euclidean vector space, as it will be shown in chapter 9

➤ **Dicke-states**

If a four particle system is described by a W_k state, it is often called *Dicke state*. So for $n = 4$ and $2 \leq k \leq 4$,

$$|W_2\rangle := \frac{1}{\sqrt{6}}(|1100\rangle + \text{Permutations}) \tag{32}$$

III Graph states

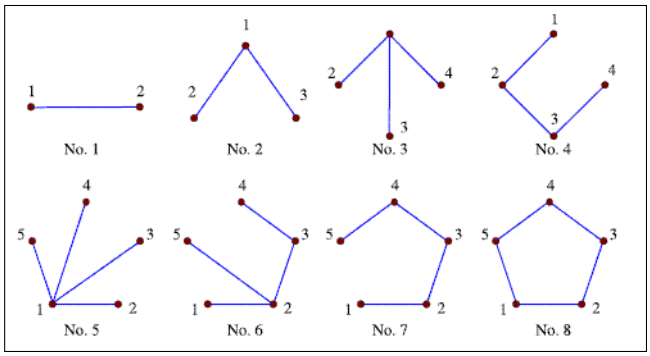


Figure 3: Graph states up to $n \leq 5$, taken from Ref. [6]

In order to introduce graph states the references [6, 14, 15] are consulted. *Graph states* are originally defined in a geometrical way, as their notation follows from a two dimensional pattern, constructed by different lines which are called *edges*. These edges are connected on so called *vertex points* and can be interpreted as the interaction between two of such vertex points, which represent quantum systems. Figure 3 shows examples of eight different possibilities of constructing such patterns for up to five particles. Hence every single vertex is connected to other adjoining vertices via edges, and all together a graph G is given by the pair $G = (V, E)$, with V being the number of vertices and E the number of edges. A more precise definition of V is given by the set that corresponds to the dimension of the system (the number of particles) $V = \{1, ..., N\}$. The number of edges E is usually specified by the set containing pairs of adjacent vertices, $E \subset [V]^2$. Considering the example of three vertices a, b and c, randomly ordered as 1, 2 and 3.

The specified sets would be $V = \{1, 2, 3\}$ and $E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$, if all vertices were connected (Triangle Graph). It has to be noted that a graph is not uniquely defined by the pair G, but with G and its associated pattern.

The actual construction of graph states can be achieved by different approaches. A quite convenient method is specifying the interactions of the edges. In the most general case the interaction between two vertices a, b is described by a unitary operator given by

$$U_{ab} = e^{-i\phi_{ab}H_{ab}}, \tag{33}$$

with H_{ab} being an interaction Hamiltonian and ϕ_{ab} the interaction strength or interaction time (e.g. for graph state $\phi_{ab} = \frac{\pi}{4}$). This unitary operator obeys $[U_{ab}U_{bc}] = 0 \; \forall a, b, c \in V$ when more than one edge is assumed as well as $U_{ab} = U_{ba}$ since the Graph is undirected (without any vertex ordering) and $U_{ab} = U$, when assuming that all vertices interact in the same way. The most studied unitaries U_{ab} are given by the so called *Ising interaction*, e.g. obtained by setting $H^I_{ab} := \sigma^a_z \sigma^b_z$. Based on this unitary operator, a graph state can be constructed:
For a given $G = (V, E)$ the graph state $|G\rangle$ is defined as

$$|G\rangle = \prod_{\{a,b\} \in E} U_{ab} \, |+\rangle^V . \tag{34}$$

By choosing $|+\rangle^V = \bigotimes_{a \in V} \left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right]^a$ (the eigenvector of σ_x to the eigenvalue $+1$) the graph state is assured to be maximally ($a = 2$) or totally entangled ($2 < a < \infty$).

The Stabilizer formalism

Another interesting way of constructing graph states leads to the so called *stabilizer formalism* of quantum states, which was originally founded for quantum error correction, i.e. regaining a desired quantum state out of a *noisy state*[19] in order to minimize

[19] A state is said to be noisy if a certain proportion α of the maximally mixed state $\mathbb{1}$ is added. Written in the density matrix form it is given as $\rho_{Noisy} = (1 - \alpha)\rho + \alpha\mathbb{1}$.

pollution effects like decoherence or channel noises [20]. For the graph state definition, it is sufficient to define stabilizers for qubits only. For this task the *generalized Pauli group* is important, which is given for an n dimensional qubit system as

$$G_n = \left\{ \begin{pmatrix} \pm 1 \\ \pm i \end{pmatrix} \sigma_{\alpha_1} \otimes ... \otimes \sigma_{\alpha_n} \right\}, \tag{35}$$

with $\alpha_k \in \{0, x, y, z\}$. G_n contains all possible "σ-combinations " for n qubits. Every element $g \in G_n$ is unitary and commutes or anti commutes pairwise. The Stabilizer group S itself is a subset of this Pauli group G_n, comprising 2^n elements and is connected with an arbitrary pure state $|\Psi\rangle$ corresponding to S. The elements of G_n and S, respectively, are restricted by the rule

$$g\,|\Psi\rangle = |\Psi\rangle\,, \tag{36}$$

i.e. S contains all eigenvectors of $|\Psi\rangle$. This means, as a result of this definition, that if g is an element of S, $-g$ is not, $g \in S \Rightarrow (-g) \neq S$. The only exception of this restriction is the negative identity operator $-\mathbb{1}$, that is never part of the Stabilizer set. It has to be noted that in order to get the minimal possible number of elements of the Stabilizer group, its elements can be reduced to at least n stabilizer generators $g_1, ..., g_n$. E.g. the identity operator $\mathbb{1}$ can be generated by σ_x^2.

For graph states, given by its pattern and $G(V, E)$, this stabilizer formalism is a helpful tool, as for every vertex j of the graph state its individual stabilizer can be constructed in the following way:

$$g_j := \sigma_x^j \bigotimes_{k=1}^{N(j)} \sigma_z^k, \tag{37}$$

with $N(j)$ denoting the number of adjoining vertices in the neighborhood of the j-th edge and σ^k denoting the acting on the k-th subsystem. Repeating this process for all vertices, a set of commuting stabilizers g_j is gained and the graph state $|G\rangle$ can be written as

$$|G\rangle\langle G| = \prod_{i=1}^{n} \frac{1}{2}(\mathbb{1} + g_i). \tag{38}$$

Using this construction the graphs in Figure 3 No. 2-4 lead to the GHZ state for 3, 4 and 5 qubits [21]. E.g. the stabilizers for pattern No.2 are given by $g_1 = \sigma_x^1 \otimes \sigma_z^2 \otimes \sigma_z^3$, $g_2 = \sigma_z^1 \otimes \sigma_x^2 \otimes \mathbb{1}_2^3$ and $g_3 = \sigma_z^1 \otimes \mathbb{1}_2^2 \otimes \sigma_x^3$.
In order to see that the stabilizer formalism is a useful tool its connection to so called *quantum circuits* is shortly sketched. Quantum circuits are basically used for the promising application of quantum computation. Furthermore they are providing another method in constructing quantum states based on the definition of special operators, the so called *Clifford gates*, that act either on single qubits or a pair of qubits, for example introduced in reference [17]. These gates are beside the Pauli operators σ_x, σ_x and

[20] Both, decoherence and channel noises, denote the fact that the time evolution of a quantum state has to be taken in account due to its interaction with its environment. The most commonly known description of such interaction is the Master or Lindblad equation, originally stated in [16].
[21] In conjunction with graph states the GHZ state is also often called star state, due to its pattern.

σ_x (19) the Hadamard gate (H), the S or Phase gate and the $CNOT$ or XOR gate, which acts on two qubits, whereas the first is called target qubit and the second control qubit. The latter three are defined as:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, \quad S = \begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix}, \quad CNOT = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}$$

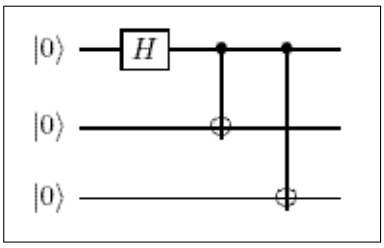


Figure 4: Quantum circuit for the 3 qubit GHZ state

The actual construction of a certain state is done by following a certain circuit, with its underlaying rules, using the above defined gates. In Figure 4 a simple three qubit circuit with the Hadamard gate H, acting on the first qubit, and two CNOT gates (given by the two vertical lines) for the subsystems $1,2$ and $1,3$, respectively. The result of this circuit is the 3 qubit GHZ state, as starting from top left $H \otimes \mathbb{1} \otimes \mathbb{1} \;|000\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\,|00\rangle$. The first CNOT applied on the control qubit and the target qubit yields $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\,|0\rangle$ and the last CNOT in the same manner on the subsystems 1 and 3 gives the GHZ state $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$.

If, however, this circuit was used with the three initial operators $A_1 := \sigma_z \otimes \mathbb{1} \otimes \mathbb{1}$, $A_2 := \mathbb{1} \otimes \sigma_z \otimes \mathbb{1}$ and $A_3 := \mathbb{1} \otimes \mathbb{1} \otimes \sigma_z$, that are the stabilizers of the $|000\rangle$ state, the resulting output operators would be $A_1' := \mathbb{1} \otimes \sigma_z \otimes \sigma_z$, $A_2' := \sigma_z \otimes \sigma_z \otimes \mathbb{1}$ and $A_3' := \sigma_z \otimes \mathbb{1} \otimes \sigma_z$. This is valid since $H\sigma_x H^\dagger = \sigma_z$, $H\sigma_y H^\dagger = -\sigma_y$ as well as $CNOT(\sigma_x \otimes \mathbb{1})CNOT^\dagger = \sigma_x \otimes \sigma_x$, $CNOT(\sigma_y \otimes \mathbb{1})CNOT^\dagger = \sigma_y \otimes \sigma_x$, $CNOT(\sigma_z \otimes \mathbb{1})CNOT^\dagger = \sigma_z \otimes \mathbb{1}$, $CNOT(\mathbb{1} \otimes \sigma_x)CNOT^\dagger = \mathbb{1} \otimes \sigma_x$, $CNOT(\mathbb{1} \otimes \sigma_y)CNOT^\dagger = \sigma_z \otimes \sigma_y$ and $CNOT(\mathbb{1} \otimes \sigma_z)CNOT^\dagger = \sigma_z \otimes \sigma_z$.

The three qubit GHZ state is an eigenstate of these resulting operators A_1', A_2' and A_3' with the eigenvalue $+1$. Furthermore all products of these new stabilizers, i.e. the operators $B_1 := -\sigma_x \otimes \sigma_y \otimes \sigma_y$, $B_2 := -\sigma_y \otimes \sigma_x \otimes \sigma_y$, $B_3 := -\sigma_y \otimes \sigma_y \otimes \sigma_x$ [22] as well as $\sigma_x \otimes \sigma_x \otimes \sigma_x$ also fulfill this property. This means that the full set of the three qubit GHZ stabilizers S contains the seven operators A_i' and B_i $(i = 1,2,3)$

$$\begin{aligned} S = \{&\sigma_x \otimes \sigma_x \otimes \sigma_x, \sigma_z \otimes \sigma_z \otimes \mathbb{1}, \sigma_z \otimes \mathbb{1} \otimes \sigma_z, \mathbb{1} \otimes \sigma_z \otimes \sigma_z,\\ &-\sigma_x \otimes \sigma_y \otimes \sigma_y, -\sigma_y \otimes \sigma_x \otimes \sigma_y, -\sigma_y \otimes \sigma_y \otimes \sigma_x\} \end{aligned} \tag{39}$$

This construction via quantum circuits can be generalized to n qubit GHZ states. Further examples are the one qubit case, with the stabilizer set $S = \{\mathbb{1}, \sigma_x\}$ and the generator $g_1 = \sigma_x$ or the two qubit case with $S = \{\mathbb{1} \otimes \mathbb{1}, \sigma_x \otimes \sigma_x, -\sigma_y \otimes \sigma_y, \sigma_z \otimes \sigma_z\}$ and its generators $g_1 = \sigma_x \otimes \sigma_x$ and $g_2 = \sigma_z \otimes \sigma_z$.

Concluding graph states, the stabilizer formalism and quantum circuits, it has to be noted that these methods not only allow a generalization of the bipartite states to more particle systems but it also denotes a complete new formalism of describing and creating

[22] Compared to the initial operators these three may be seen as the inverse operators, as $\mathbb{1}$ and σ_z is exchanged.

states that can be useful to understand certain symmetries or connections to other states as well as their corresponding entanglement properties. For more results or applications it is referred to chapter 6.2 or the references [18, 17].

For more interesting results depending the different kinds of entanglement of states it is referred to [19], in which the authors have shown a few of the differences of these states with the help of a constructed measure, based on the terms described in chapter 7.

Part II
Characterization of Separable and Entangled States

CHAPTER 3

Bell inequality

3.1 Locality and HVT-Theories

Bell inequalities are one of the oldest method of classifying quantum states. When putting it into its historical concept the work of Einstein, Podolsky and Rosen from 1935 has to be considered, in which the question is asked whether the *Quantum-Mechanical Description of Physical Reality [Can] Be Considered Complete?* [20]. In this paper, which is often referred to as the *EPR-Paradox*, the following presumptions are introduced:

- **Completeness:**

  'Every element of the physical reality [23] *must have a counterpart in the physical [quantum] theory.'.*

- **Reality:**

  'If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity.'

Furthermore Einstein et al. assumed a Gedankenexperiment, in which a bipartite state Ψ is given, whose two subsystems (Alice and Bob) are allowed to interact in between the time interval $t = 0$ to a certain time T. For any further time $t > T$, when no interaction is allowed, the time evolution of the combined state can be described by the Schrödinger equation. When assuming an hermitian operator A with its corresponding eigenvalues (observables) $a_1, a_2, \ldots$ and eigenfunctions $u_1(x_A), u_2(x_A), \ldots$ the combined state Ψ can be written as

$$\Psi(x_A, x_B) = \sum_{n=1}^{\infty} \Psi_n(x_B) u_n(x_A), \tag{40}$$

with x_A and x_B being the variables used by Alice and Bob, respectively, and the functions $\Psi_n(x_B)$ acting as the coefficients of the state expressed in a series of eigenfunctions of $u_n(x_A)$, with respect to Bob´s subsystem. If furthermore the observable a_k on a time $t > T$ was measured, the state would reduces to $\Psi_k(x_B)u_k(x_A)$.

Considering now the same situation, however altering the operator A to another hermitian operator B, with its corresponding observables $b_1, b_2, \ldots$ and eigenfunctions $v_1(x_A), v_2(x_A), \ldots$. Supposing again the measurement of the l-th observable at a time $t > T$, the remaining state is then given by $\phi_l(x_B)v_l(x_A)$.

[23] This means for quantum mechanics: every measurement result of an observable.

Combining the above introduced definitions of reality and completeness and assuming that the two operators A and B are non-commuting, i.e. $AB \neq BA$ [24], a contradiction to the assumed definitions can be deduced, since the state of the second subsystem is once given by $\Psi_k(x_B)$, another time by $\phi_l(x_B)$, depending on the eligible observable measured by Alice. However since this measurement is considered at the time $t > T$ and no interaction between the two subsystems is allowed, it is possible to assign two different wave functions to the same reality. This argument is commonly called *local reality* (or *Locality*) [25].
The contradiction is now received, when Alice measures her observable, as it now can be predicted (with probability 1) in which eigenstate Bob´s system is (without disturbing it). That means that with Bob´s system being in a defined state and Alice´s measured observable, the uncertainty principle of two non-commuting observables is violated and at least one of the introduced assumptions can not be valid.

The authors of this paradox deduced that the description of a quantum state via wave functions is insufficient and hence the quantum theory is incomplete, however keeping the option of a complete theory open.
This statement was criticized by others (especially by Niels Bohr), claiming that the introduced assumption of locality is no valid approach.

With this Paper Einstein et al. initiated the theory of hidden variables (HVT), that were introduced in order to restore the completeness of quantum mechanics and solve the EPR-paradox. Although it is not fully clarified whether Einstein was propagating such hidden variables, HVT are able to bring determinism back into quantum theory by claiming, that the result of a measurement is pre-existing at any time in terms of a variable λ, which can not be determined. Considering for example an observable with its associated hermitian operator A, the hidden variable λ can be introduced as a function of this operator $A(\lambda)$, in such a way that the predictions of quantum theory are reproduced properly.
The reason why all HVT are in general disproved is the fact that they can be deduced to a contradiction using the very axioms of these theories itself, namely locality as well as non-contextuality. The latter presupposition, which means that the measurement results depend on the measurement itself and the assembling of the measurement device, respectively, leads to a contradiction found by van Neumann [21] or later by the Kochen and Specker in their theorem [22]. However the most famous disproof of hidden variable theories was found by John Bell, which will be explicitly shown in the next chapter.

Hence up to now the EPR-Paradox and the interpretation, of the formalism of quantum mechanics can not be solved and leaves the rather philosophical question of interpretation behind. Beside the popular Kopenhagen interpretation other approaches such as Everett [23], Penrose [24] and Bohmian quantum mechanics [25, 26, 27] shall be mentioned shortly and can be investigated further using the respective references.

3.2 Bell and CHSH inequality

After a long argue about whether quantum mechanics can be expressed via hidden variables, John Bell derived an astonishing answer to this question. He claimed in his work [28], that if a HVT existed, it would be possible to solve this problem by simply performing the

[24] This is shown explicitly in [20] for A, B being the position and momentum operator, $[X, P] = -i\hbar$.
[25] As the lack of interaction is usually referred to a spatial separation, local reality is often described by, *'no action at distance'*.

proposed Gedankenexperiment of Einstein et al. . In the following picture the set up of this experiment is shown, which was experimentally first realized with a pair of entangled photons with different polarizations, here denoted by 0 and 1 (i.e. measurement of the non-commuting spin observables).

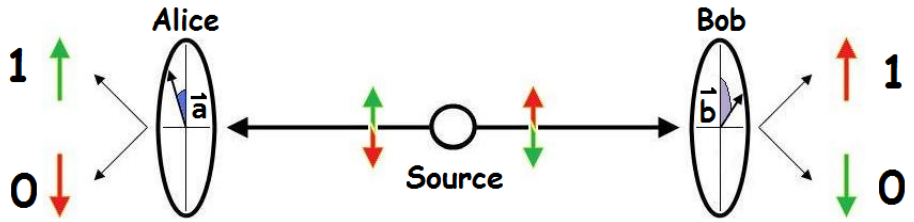


Figure 5: Experimental set up for detecting the correlation of entangled photons

When regarding the expectation value of the joint spin measurement results of both parties, it must be possible to see when a correlation (or anti-correlation) of the measurement results occurs. This correlation depends on the angle between the directions $\vec{a}$ and $\vec{b}$, as the expectation value of the two spin operators $\vec{\sigma}_A$ and $\vec{\sigma}_B$ for a singlet state (e.g. the Bell state $|\Psi^+\rangle$) yields $E(\vec{a},\vec{b}) = \left\langle \Psi^+|\vec{\sigma}_A\vec{a}\otimes\vec{\sigma}_B\vec{b}|\Psi^+\right\rangle = -\vec{a}\cdot\vec{b} = -cos(\psi)$, with ψ being the angle between $\vec{a}$, $\vec{b}$ and $\left|\vec{a}\right| = \left|\vec{b}\right| = 1$.

In the following Bell introduces the hidden variable λ with the property $\int \rho(\lambda)d\lambda = 1$, whereas $\rho(\lambda)$ denotes the distribution over the probability space (normalization) [26]. The hidden variable should reproduce the above calculated value however assuming now local realism. Together with the directions, λ is aligned to the eligible outcomes of the two spin measurement results A and B, namely $A(\vec{a},\lambda) = \pm 1$ for Alice and $B(\vec{a},\lambda) = \pm 1$ for Bob. The expectation value of the combined measurement of the two observables now yields

$$E(\vec{a},\vec{b})_\lambda = \int A(\vec{a},\lambda)B(\vec{b},\lambda)d\lambda. \tag{41}$$

For further calculations $A(\vec{a},\lambda) = -B(\vec{b},\lambda)$ is assumed, which is equivalent to a perfect anti-correlation of the measurement results of Alice and Bob, i.e. the measurement directions $\vec{a}$ and $\vec{b}$ are parallel (compare the above expectation value: $E(\vec{a},\vec{b}) = -1 \rightarrow \psi = 0$):

$$E(\vec{a},\vec{b})_\lambda = -\int A(\vec{a},\lambda)A(\vec{b},\lambda)d\lambda \tag{42}$$

When introducing another unit vector $\vec{c}$ and calculating the difference of this expectation value with $E(\vec{a},\vec{c})_\lambda$, one receives, respecting the fact that $A(\vec{b},\lambda)^2 = \pm 1^2 = 1$,

$$\begin{aligned} E(\vec{a},\vec{b}) - E(\vec{a},\vec{c}) &= -\int A(\vec{a},\lambda)A(\vec{b},\lambda) - A(\vec{a},\lambda)A(\vec{c},\lambda)d\lambda, \\ E(\vec{a},\vec{b}) - E(\vec{a},\vec{c}) &= \int A(\vec{a},\lambda)A(\vec{b},\lambda)\left[A(\vec{b},\lambda)A(\vec{c},\lambda) - 1\right]d\lambda. \end{aligned} \tag{43}$$

[26] W.l.o.g. λ is considered as a single continuous parameter.

Using the absolute value and the triangle inequality, it yields

$$\begin{aligned}\Big|E(\vec{a},\vec{b}) - E(\vec{a},\vec{c})\Big| &= \left|\int A(\vec{a},\lambda)A(\vec{b},\lambda)\Big[A(\vec{b},\lambda)A(\vec{c},\lambda) - 1\Big]\,d\lambda\right| \\ &\leq \int \Big[1 - A(\vec{b},\lambda)A(\vec{c},\lambda)\Big]\,d\lambda\end{aligned} \tag{44}$$

According to equation (43) this is

$$\Big|E(\vec{a},\vec{b}) - E(\vec{a},\vec{c})\Big| \leq 1 + E(\vec{b},\vec{c}), \tag{45}$$

which is the original form of the inequality, that was found by Bell. This inequality is violated by inserting certain directions $\vec{a}, \vec{b}$ and $\vec{c}$ and calculating their individual expectation values for certain quantum states. This means furthermore that the predictions of quantum mechanics can not be reproduced by adding hidden variables without violating local reality. Another possibility of saving the axiom of Locality is discarding the assumption of reality, that was introduced in the previous section. However, this is commonly not the case.
In order to prepare this result for experimental purposes, the perfect correlations of probabilities, as it was assumed by Bell, can of course not be reached ($E(\vec{a},\vec{b}) = -1$). Therefore a derivation of this theorem was introduced by Clauser, Horne, Shimony and Holt, the so called *CHSH inequality*, in order to confirm Bell´s theorem on a more 'experimental-friendly' way. Beside $E(\vec{a},\vec{b}) = -1+\delta$, with $\delta > 0$ and taking the mean values of a suitable number of measurements, which is in the following denoted by $\bar{A}$ and $\bar{B}$, respectively, it is also assumed that the observables $A(\vec{a},\lambda)$ and $B(\vec{a},\lambda)$ can take the values $\{-1,0,1\}$, with 0 being the result of ´no detection'.

Considering now again the difference of the two expectation values $E(\vec{a},\vec{b}) - E(\vec{a},\vec{c})$ (see equation (44)) one receives

$$\begin{aligned}E(\vec{a},\vec{b}) - E(\vec{a},\vec{c}) &= \int \big(\bar{A}(\vec{a},\lambda)\bar{B}(\vec{b},\lambda) - \bar{A}(\vec{a},\lambda)\bar{B}(\vec{c},\lambda)\big)\rho(\lambda)d\lambda \\ &= \int \bar{A}(\vec{a},\lambda)\bar{B}(\vec{b},\lambda)\big(1 \pm \bar{A}(\vec{a}',\lambda)\bar{B}(\vec{c},\lambda)\big)\rho(\lambda)d\lambda - \int \bar{A}(\vec{a},\lambda)\bar{B}(\vec{c},\lambda)\big(1 \pm \bar{A}(\vec{a}',\lambda)\bar{B}(\vec{b},\lambda)\big)\rho(\lambda)d\lambda,\end{aligned} \tag{46}$$

with $\vec{a}'$ being again a unit vector representing a measurement direction. Proceeding as before with the absolute value and the triangle inequality, it follows that

$$\Big|E(\vec{a},\vec{b}) - E(\vec{a},\vec{c})\Big| \leq 2 \pm \big(E(\vec{a}',\vec{c}) + E(\vec{a}',\vec{b})\big). \tag{47}$$

The primal example of this set up is, as mentioned before, the bipartite quantum state of two spin $\frac{1}{2}$-particles. I.e. rewriting A and B in terms of the Pauli spin matrices the CHSH-operator can be defined as

$$\mathcal{B}_{\text{CHSH}} := A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2), \tag{48}$$

with $A_i = \vec{a}_i \cdot \vec{\sigma}$ and $B_i = \vec{a}_i \cdot \vec{\sigma}$ for $i = 1,2$. Using this the inequality can furthermore be written in an operator valued form,

$$\big|Tr\big(\mathcal{B}_{\text{CHSH}}\rho\big)\big| \leq 2, \tag{49}$$

which shows in a more explicit way the constraint that has to be fulfilled by a quantum state ρ. It again turns out that not all states fulfill the CHSH, just like the previous version of

the Bell inequality. For a certain class of entangled states this theoretical bound is violated, especially for the $|\Psi^-\rangle$ Bell state one can find the maximal violation of $2\sqrt{2}$, shown in reference [29]. It can be shown further that every pure bipartite states violates a Bell inequality, but the existence of a single Bell inequality, which is violated by all entangled states is not valid. Such a dependence of a criterion on a state is a common situation and is for instance also for entanglement witnesses. This leads to the assumption, that Bell inequalities and entanglement witnesses are somehow connected. For more precise investigations in this directions it is referred to chapter 8.3. Furthermore it is shown that a impurity of white noise, that is added to a pure entangled state can still violate the CHSH inequality up to a certain level: i.e. a given state $\rho := p\,|\Psi^-\rangle\langle\Psi^-| + (1-p)\mathbb{1}$ is nonlocal for $p > \frac{1}{\sqrt{2}}$ [27]. This becomes an important issue for the experimental task, where creating a pure entangled state is impossible. A state violating a Bell inequality is said to be nonlocal, but in general it is hard to discriminate whether a state has nonlocal properties or not, since up till now plenty of different forms of Bell inequalities are found and also for higher dimensions generalization to more particles and/or more degrees of freedoms open the range for new constructions. Whether a state is entangled or not is a sufficient criterion for violating a Bell inequality. This means that a bipartite state violating a Bell inequality is (beside being nonlocal) also an entangled state, whereas the reverse statement is not valid for all states. The violation of a Bell inequality can be used in order to give a sufficient indication of a state to be entangled. For multipartite states a similar result can be posed and is introduced in the next section.

3.3 Generalizations to multipartite qubits

In principal the method of Bell´s theorem is easy to generalize for n-partite systems by defining the probability in analogy to equation (40) [6]

$$P(a_i, b_j, c_k, ...) = \int \bar{A}_i(\lambda)\ \bar{B}_j(\lambda)\ \bar{C}_k(\lambda)\ ...\ \rho(\lambda)d\lambda, \tag{50}$$

with n observables, written in capital letters, and their corresponding measurement results, given in lower case letters. Considering now all possible factorizations of a state ρ (i.e. the k-separability, eq. (28)) the probabilities of two measurement results have to be chosen in a similar way in order to receive a proper Bell inequality which makes sure that all nonlocal properties between all subsystems are regarded. E.g. for $n = 3$ all bipartite cuts have to be considered,

$$P(a_i, b_j, c_k) = \int \bar{A}_i(\lambda) \underbrace{\bar{O}_l}_{B_j, C_k} \rho_O(\lambda)d\lambda + \int \bar{B}_i(\lambda) \underbrace{\bar{P}_l}_{A_j, C_k} \rho_P(\lambda)d\lambda + \int \bar{C}_i(\lambda) \underbrace{\bar{Q}_l}_{A_j, B_k} \rho_Q(\lambda)d\lambda, \tag{51}$$

with $\int \rho_O(\lambda)d\lambda + \int \rho_P(\lambda)d\lambda + \int \rho_Q(\lambda)d\lambda = 1$. Following the method of CHSH inequality, that used two observers with two outcomes on each party, the best known n partite Bell inequality with this respective setting is the so called *Mermin* inequality defined by the Bell operator B_{Mermin}

$$\begin{aligned} B_{\text{Mermin}} &:= X_1X_2X_3X_4... - Y_1Y_2X_3X_4... + Y_1Y_2Y_3Y_4... - +... \\ &= \sum_{\pi} X_1X_2...X_n - \sum_{\pi} Y_1Y_2X_3...X_n - ... + ..., \end{aligned} \tag{52}$$

[27] For this state the ppt criterion yields $p > \frac{1}{3}$ as the border between SEP and the set of entangled states

whereas $\sum_\pi$ denotes the permutation of all observables. The analogy to the CHSH inequality is given by choosing X, Y as σ_x,σ_y, whereas for this choice the maximal violation is achieved for GHZ states. In a similar way more Mermin-like inequalities can be constructed. Also another construction could be found, that includes all these types and is therefore a more general construction for higher dimensional cases and multi-particles problems.
The inequality given by

$$B_{\text{Ardehali}} := \left\langle (A_1^+ - A_1^-)(-\sum_\pi X_2X_3...X_n + \sum_\pi Y_2Y_3X_4...X_n - ... + ...)\right\rangle + \tag{53}$$
$$\left\langle (A_1^+ + A_1^-)(\sum_\pi Y_2X_3...X_n - \sum_\pi Y_2Y_3Y_4X_5...X_n + \sum_\pi X_2Y_3Y_4Y_5Y_6X_7...X_n - ... + ...)\right\rangle \leq 2^{\frac{n}{2}},$$

with $A_1^\pm := \frac{(\mp X_1 - Y_1)}{\sqrt{2}}$ and $\sum_\pi$ being again the permutation over all observables, is called Ardehali inequality and has a slightly different construction compared to the previous Mermin inequality, e.g. the base change for X_1 and Y_1. The exact theory can be found in [30]. Without going further into details the only difference to the Mermin inequality is given by using non stabilizer operators, i.e. the operators are not in the same eigenspace as the states are. This however leads to the fact, that more states can be found violating this inequality.

CHAPTER 4

Peres-Horodecki criterion

This criterion was first established in 1996 by Asher Peres and is a far stronger condition compared to Bell-inequalities when it comes to detecting whether a bipartite state is entangled or not. A quantum system consisting of two subsystems is separable if its density matrix can be written as $\rho = \sum_i p_i \ \rho_A^i \otimes \rho_B^i$, where ρ_A^i and ρ_B^i are density matrices of pure states of the two subsystems. Asher Peres showed in his paper [31] that a necessary condition for separability of an arbitrary mixed bipartite state is obtained by verifying that the so called *partial transposition* of its density matrix ρ, has only non-negative eigenvalues.
The exact definition is given as follows:

Definition (partial transposition (pt)):
For $|e_i\rangle$ and $|b_i\rangle$ being base vectors for $\mathcal{H}_A$ and $\mathcal{H}_B$, the partial transposition of a bipartite state, given by the density matrix ρ, with its elements

$$\rho_{m\mu,n\nu} = \langle e_m \otimes b_\mu | \, \rho \, | e_n \otimes b_\nu \rangle \, , \tag{54}$$

is defined as

$$\rho^{T_B}_{m\mu,n\nu} = \rho_{m\nu,n\mu}. \tag{55}$$

Due to $\rho^{T_A} = (\rho^{T_B})^T$ an equivalent definition can be posed by changing the indices of the first subsystem. With this definition the criterion can now be introduced:
Proposition (pt criterion)[28]:
A state ρ is separable if the partial transposed Matrix σ^{T_B} is again a valid density matrix (i.e. a non negative matrix with trace one).
Proof:
Considering a separable bipartite state ρ, written as $\rho = \sum_i p_i \ \rho_i^A \otimes \rho_i^B$. After its the partial transposition it is turned into the state $\rho^{T_B} = \sum_i p_i \ \rho_i^A \otimes (\rho_i^B)^{T_B}$. This is nothing else than applying the operator $\mathbb{1} \otimes T$ on ρ with T being the transposition operation: $(\mathbb{1} \otimes T)(\rho) = \rho^{T_B}$. As long as T is a positive map and ρ a density matrix the transposed state ρ^{T_B} is also again a density matrix (i.e. all eigenvalues must be greater or equal 0 and $Tr(\rho) = 1$). That means on the other hand that if ρ^{T_B} contains negative eigenvalues the original state ρ can not be written as a separable density matrix and therefore must be entangled.
Hence the positivity of the partial transposition of a separable matrix is a sufficient property and also a necessary criterion for bipartite systems with dimensions $\mathcal{H}_A^2 \otimes \mathcal{H}_B^2$ and $\mathcal{H}_A^2 \otimes \mathcal{H}_B^3$. However for higher dimensional states as well as for multipartite systems the positivity of the partial transposed states turns out to be no more sufficient, but certainly necessary.

In order to show why this criterion is no more sufficient for higher dimensions, a more precise approach to this criteria has to be made following the original work of Peres as well as the further investigations of Horodecki´s et al. [32]. The first step is done by introducing a set of maps $L(\mathcal{B}(H_A), \mathcal{B}(H_B))$, that comprises all maps leading from the set of bounded operators acting on H_A, denoted by $\mathcal{B}(H_A)$, to the set of bounded operators acting on H_B, denoted by $\mathcal{B}(H_B)$.

[28] It is often also called Peres-Horodecki criterion

Furthermore such a map $\Lambda \in L(A_1, A_2)$ is called a positive map, iff a positive operator of $\mathcal{B}(H_A)$ is again mapped into a positive operator of $\mathcal{B}(H_B)$, i.e. $\Lambda(\mathcal{B}(H_A)) = \mathcal{B}(H_B) \geq 0$ (compare chapter 1).
As a consequence of the Hahn-Banach theorem, see e.g. [33], it can be proposed that the convex set of separable states SEP and inseparable states ISEP can be strictly divided by some Hermitian operator A [29] such that

$$Tr(A\rho) \geq 0 \quad \text{for} \quad \rho \in SEP \tag{56}$$
$$Tr(A\tilde{\rho}) < 0 \quad \text{for} \quad \tilde{\rho} \in ISEP. \tag{57}$$

The separability of bipartite systems can therefore be expressed by using an Hermitian operator $\tilde{A} \in \mathcal{B}(H_A) \otimes \mathcal{B}(H_B)$:

$$\rho \in \mathcal{H}_A \otimes \mathcal{H}_B \text{ is separable } \Leftrightarrow Tr\tilde{A}\rho \geq 0, \quad \text{with } Tr(\tilde{A}(P_A \otimes P_B)) \geq 0, \tag{58}$$

with $P_{A/B}$ being the projectors on the A/B-th Hilbert space $\mathcal{H}_{A/B}$. This formalism can be generalized straightforward to higher dimensions (more degrees of freedom).

The fundamental task of explaining how this pt-criterion works in a mathematical way is finding an isomorph relation S between the previously introduced set $L(A_1, A_2)$ and the very operators of $\mathcal{B}(H_A)$ and $\mathcal{B}(H_B)$ itself.

$$S: \ \Lambda \in L(A_1, A_2) \rightarrow \tilde{A} \in \mathcal{B}(H_A) \otimes \mathcal{B}(H_B) \tag{59}$$

It can be shown [34], that $S(\Lambda)$ is a Hermitian and positivity preserving as well as an isomorphic relation (with respect to an inner product) and it can be expressed as $S(\Lambda) = \sum_i E_i^\dagger \otimes \Lambda(E_i)$, with $\{E_i\}$ being an orthogonal operator base of $\mathcal{H}_A$. This is used to verify the following theorem.

Theorem 1
$\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$ is separable, iff for any positive map $\Lambda \in L(A_1, A_2)$ the operator $(\mathbb{1} \otimes \Lambda)(\rho)$ is positive.

Proof:
Assuming $S(\Lambda) = \sum_{i,j} P_{ij}^\dagger \otimes \Lambda(P_{ij})$, with $P_{ij} = |i\rangle \langle j|$ being a set of orthogonal projectors referred to an orthonormal base $\{e_i\}$ ($P_{ij}e_k = \delta_{ik}$) and fulfilling $\sum_{i,j \leq n} P_{ij}$, with $n = dim H_A$, equation (53) can be rewritten as

$$Tr(\rho S(\Lambda)) = Tr\left\{[(\mathbb{1} \otimes \Lambda) \sum_{i,j} P_{ji} \otimes P_{ij}]\rho\right\} \geq 0 \tag{60}$$

$$\Rightarrow Tr\left\{[(\mathbb{1} \otimes \Lambda T) \sum_{i,j} P_{ji} \otimes TP_{ji}]\rho\right\} \geq 0, \tag{61}$$

while T is the transposition map, which is not only a projector ($T^2 = 1$) but also positive with respect to the base e_i of $\mathcal{H}_A$.
Rewriting this condition by defining the hermitian operator $P_0 := \frac{1}{n} \sum_{i,j} P_{ji} \otimes P_{ji}$ and replacing the trace by the scalar product gives

$$\left\langle \rho, (\mathbb{1} \otimes \Lambda P_0)^\dagger \right\rangle. \tag{62}$$

[29] Such an operator is called an entanglement witness and will be investigated further in chapter 8.

Since T preserves the property of the operator P_0 being hermitian and Λ is a positive map, it is equivalent to write

$$\langle \rho, (\mathbb{1} \otimes \Lambda P_0) \rangle = \langle (\mathbb{1} \otimes \Lambda)\rho, P_0 \rangle = Tr((\mathbb{1} \otimes \Lambda^\dagger)\rho P_0) \tag{63}$$

As $(\mathbb{1} \otimes \lambda^\dagger)$ is a positive map, the desired result is gained by regarding iff $(\mathbb{1} \otimes \lambda^\dagger)$ is positive:

" $\Rightarrow$ " ρ is separable $\Rightarrow (1 \otimes \Lambda)\rho$ is positive for any positive $\Lambda \Rightarrow Tr((\mathbb{1} \otimes \Lambda^\dagger)\rho P_0) \geq 0$

" $\Leftarrow$ " $\mathbb{1} \otimes \Lambda\rho$ is positive $\Rightarrow Tr((\mathbb{1} \otimes \Lambda^\dagger)\rho P_0) \geq 0 \Rightarrow$ with Equation (56) ρ is separable.

With the help of theorem 1 one can propose another theorem, that is equivalent to the ppt criterion formulated at the beginning of this chapter, but with the difference that it is now able to see why the positive partial transposition is no longer a necessary property for higher dimensions:

Theorem (pt)
A state ρ is separable if its partial transpose, $\rho^{T_B} = (1 \otimes T)(\rho)$, is a positive operator. If $\rho \in {\mathcal{H}_\mathcal{A}}^2 \otimes {\mathcal{H}_\mathcal{B}}^2$ or ${\mathcal{H}_\mathcal{A}}^3 \otimes {\mathcal{H}_\mathcal{B}}^2$ the inverse statement is also true (if $\rightarrow$ iff), i.e. it is a necessary and sufficient criterion.

Proof:
"$\Rightarrow$ " If ρ is separable ρ^{T_2} is a positive operator.
"$\Leftarrow$ " In order to show the backwards direction one starts from the opposite, i.e. ρ^{T_B} is assumed to be positive operator. It is shown in [35], that every positive map $\Lambda \in L(\mathcal{B}(H_A), \mathcal{B}(H_B))$, that acts on ${\mathcal{H}_\mathcal{A}}^2 \otimes {\mathcal{H}_\mathcal{B}}^2$ or ${\mathcal{H}_\mathcal{A}}^3 \otimes {\mathcal{H}_\mathcal{B}}^2$ can be expressed with the help of a completely positive maps Λ_i^{CP} and the transposition operator T as

$$\Lambda = \Lambda_1^{CP} + \Lambda_2^{CP} T. \tag{64}$$

Because of $\Lambda_i = 1 \otimes \Lambda_i^{CP}$ being a positive map due to the fact that Λ_i^{CP} is a completely positive one, one can connect to theorem 1 ("$\Leftarrow$ ") as it is proved analogously. As this construction (62) of a positive map is no longer valid for higher dimensional operators, the pt criterion is no longer a necessary property. This fact is shown more precise formulated in the following way:

For higher dimensional density operators ρ [30] this criterion works only as a necessary criterion because equations (54) and (55) do not hold strictly. In order to see where the proof fails one has to compare the set of positive operators that remains positive after partial transposition $S_T := \left\{A \in A_1 \otimes A_2 : A \geq 0, A^{T_2} \geq 0\right\}$ and the set of all separable states $S := \{\lambda\rho : \lambda \geq 0,\ \rho \text{ separable}\}$. These turn out not to be equal which can be seen by taking the dual sets, i.e. positive linear functionals of both sets, whereas the dual set of S is isomorph to all positive maps and the dual set of S_T is given by

$$W_T = \left\{Tr[A\,\cdot] : A = B + C^T, \text{ with } B,\ C \text{ being a positive operators}\right\}, \tag{65}$$

which equals the cone of maps of equation (62). However this equation does not hold for higher dimensions. Therefore this criterion is not longer sufficient for higher dimensional cases.

[30] Higher dimensional means that either the degree of freedom of of the particles is increased or the number of particles or both.

CHAPTER 5

Realignment criterion

Similar to PT-criterion the so called *realignment criterion* has been established due to its easiness and handy application for pure and mixed states of bipartite systems of arbitrary dimension. In reference [36] it is shown that is closely related to the theory of Schmidt coefficients (SC), which are defined for a pure bipartite state $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ as the square roots of the corresponding coefficients to a common decomposition of the two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. Although this is already shortly sketched in the first chapter of this thesis a more precise definition in a more useful form for the realignment criterion is stated in the following.

Definition(Schmidt-decomposition):
An arbitrary bipartite density operator ρ can always be written as

$$\rho = \sum_{i=1}^{d} \lambda_i \; F_A^i \otimes F_B^i \qquad \text{with} \quad \lambda_1 \geq \lambda_2 \geq ... \geq \lambda_d \geq 0 \tag{66}$$

whereas the hermitian, orthonormal operators $F_{A/B}^i$ are elements of an operator base on $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_{A/B})$[31], with

$$Tr[F_A^j F_A^k] = Tr[F_B^j F_B^k] = \delta_{jk} \qquad \text{for} \quad j,k \in \{1,2,...,d\}\,. \tag{67}$$

Therefore at most $d = min\,\{dim\mathcal{H}_A, dim\mathcal{H}_B\}$ different Schmidt coefficients λ_i exist.
Based on this fact, the following Theorem already gives a necessary condition for separability.

Theorem
It can be shown [36], that a density operator ρ is separable if its Schmidt-coefficients fulfill

$$\sum_{i}^{d} \lambda_i \leq 1 \tag{68}$$

This result can actually be seen as the realignment criterion itself, however another formulation of the criterion can be stated which allows an easy calculation of the left hand side of equation (66) by reordering the matrix coefficients of the density matrix.

Theorem (Realignment criterion for separability):
Considering a bipartite mixed or pure state with its density matrix $\rho_{m\mu,n\nu}$ represented in an arbitrary but fixed orthonormal product basis, compound by the bases of $\mathcal{H}_A$ ($|m\rangle$ and $|n\rangle$) and $\mathcal{H}_B$ ($|\mu\rangle$ and $|\nu\rangle$, respectively), i.e. $\rho_{m\mu,n\nu} = \sum_{m,\mu,n,\nu} c_m c_\mu c_n^* c_\nu^* \,|m\mu\rangle\langle n\nu| = \sum_{m,\mu,n,\nu} \tilde{c}_{m\mu n\nu} \,|m\mu\rangle\langle n\nu|$. A new matrix ρ^R can be received by realigning its elements $\tilde{c}_{m\mu n\nu}$ in the following way

$$\rho^R_{mn,\mu\nu} := \rho_{m\mu,n\nu}. \tag{69}$$

Via singular value decomposition this matrix can be written as

$$\rho^R = \mathcal{U} D \mathcal{V}, \tag{70}$$

[31] $\mathcal{L}_{\mathbb{R}}(\mathcal{H}_{A/B})$ denotes the real vector space of all operators mapping from $\mathcal{H}_{A/B}$ to $\mathcal{H}_{A/B}$. However ρ itself is an element of a subset of the composed set $L(\mathcal{H}) = \mathcal{L}_{\mathbb{R}}(\mathcal{H}_A) \otimes \mathcal{L}_{\mathbb{R}}(\mathcal{H}_B)$, because of the $Tr\,[\rho] = 1$ condition.

with D being a diagonal, rectangular matrix in dependence of the unitary matrices $\mathcal{V}$ and $\mathcal{U}$ of the unitary groups of their corresponding subsystem $U(N_A^2)$ or $U(N_B^2)$. The entries of D along its diagonal are the singular values of the realigned matrix ρ^R. It can be shown further that, according to the previous construction, theses singular values are the SC of the original matrix ρ. A necessary condition for the separability of ρ is therefore obtained by fulfilling (66). If the special case is contemplated, in which the singular values of are nothing else but the eigenvalues ρ^R this condition can be written by using the trace-norm [32] of the realigned matrix,

$$\left\|\rho^R\right\|_{\mathrm{Tr}} := Tr[\sqrt{\rho^R\,{}^{\dagger}\rho^R}] \leq 1. \tag{71}$$

An exact proof of this theorem is given in the next section.
However a small drawback of this criterion has to be noted: The characterization of a state by its Schmidt coefficients is not unique, i.e. a single set of SC can be assigned to more than one state. Therewith different equivalence classes of states are constructed corresponding to a certain set of SC, for which different properties can be determined. For more information it is referred to reference [36]

5.1 Realignment criterion via matrix analysis

For completeness, an older construction, inspired by basic matrix analysis, found by Kai Chen et al. [37], will now be stated. It is more helpful for special application, when it comes to computing the actual realigned matrix or its norm. First of all a general definition has to be introduced for an arbitrary $m \times n$ matrix $\mathbf{A} = (a_{ij})$, $i \in \{1, ..., m\}, j \in \{1, ..., n\}$, whose elements are transformed into a vector by the following map:

$$vec(\mathbf{A}) := \left[a_{11}, ...a_{m1}, a_{12}, ..., a_{m2}, ..., a_{1n}, ..., a_{mn}\right]^T \tag{72}$$

Due to the properties of the Kronecker Product the following identities for $vec(\cdot)$ for arbitrary block matrices X, Y and Z are valid:

$$vec(XYZ) = (Z^T \otimes X)vec(Y) \tag{73}$$

$$Z = X \otimes Y \Leftrightarrow Z^R = vec(X)vec(Y)^T \tag{74}$$

It turns out that this map is quite useful whenever the realigned version of a $m \times m$ matrix $\mathcal{M}$ has to be determined. As density operators are the matrices of interest, the restriction to symmetric matrices is valid. Hence the matrix $\mathcal{M}$ can always be divided into $(\frac{m}{n})^2$ block-submatrices $\Omega_{i,j}$, with $i, j \in \left\{1, 2, ..., \frac{m}{n}\right\}$, each of the size n, as long as n is chosen to be a divider of m (also this is no restriction for quantum states). I.e. The $m \times m$ decomposition and as an example the first $n \times n$ submatrix $\Omega_{1,1}$ is given by

$$\mathcal{M} = \begin{pmatrix} \Omega_{11} & \Omega_{21} & \cdots & \Omega_{\frac{m}{n}1} \\ \Omega_{12} & \ddots & & \vdots \\ \vdots & & & \\ \Omega_{1\frac{m}{n}} & \cdots & & \Omega_{\frac{m}{n}\frac{m}{n}} \end{pmatrix}, \quad \text{with} \quad \Omega_{1,1} = \begin{pmatrix} m_{11} & m_{21} & \cdots & m_{n1} \\ m_{12} & \ddots & & \vdots \\ \vdots & & & \\ m_{1n} & \cdots & & m_{nn} \end{pmatrix} \tag{75}$$

[32] In the general case for singular values the Trace Norm is also often called the Ky Fan norm.

and in the same manner the other $\Omega_{i,j}$ sub-matrices. With this decomposition the realigned matrix is given by

$$\mathcal{M}^R := \begin{pmatrix} vec(\Omega_{1,1})^T \\ \vdots \\ vec(\Omega_{\frac{m}{n},1})^T \\ \vdots \\ vec(\Omega_{1,\frac{m}{n}})^T \\ \vdots \\ vec(\Omega_{\frac{m}{n},\frac{m}{n}})^T \end{pmatrix} \tag{76}$$

The resulting realigned matrix is of the size $\frac{m}{n} \times n$, which shows that all elements of the original matrix are comprised in a reordered way. Again reminding the connection to the generalized Schmidt-coefficients in comparison with this construction, a slightly different formulated theorem, however with the same statement as in the previous section, can be posed.

Theorem (Realignment criterion):
If a bipartite $m \times n$ density operator ρ_{AB} is separable, it follows that the trace norm of the singular values of the realigned $m^2 \times n^2$ matrix ρ_{AB}^R is less than 1,

$$\left\|\rho_{AB}^R\right\|_{\mathrm{Tr}} = \sum_{i=1}^{s} \lambda_i \leq 1. \tag{77}$$

The sum runs over all $s = \min\{m^2, n^2\}$ singular values λ_i of ρ_{AB}^R.
Based on this matrix analysis the proof of this theorem is done rather quickly by using the properties of the Kronecker product.
Proof:
Assuming the separable state ρ_{AB}, that is expressed by U_A^i and U_B^i, the two unitary operators diagonalizing the respective subsystems ρ_A and ρ_B, as well as $E_{ij}^{k,l}$, a $k \times l$ matrix with the single entry 1 for the ij-th element and otherwise 0:

$$\rho_{AB} = \sum_i p_i \ \rho_A^i \otimes \rho_B^i = \sum_i p_i \ (U_A^i \ E_{11}^{m,m} \ (U_A^i)^\dagger) \otimes (U_B^i \ E_{11}^{n,n} \ (U_B^i)^\dagger) \tag{78}$$

Using the properties of the $vec(\ )$ map (71) and (72) the realigned matrix of $\rho_{AB} = \sum_i p_i \ \rho_A^i \otimes \rho_B^i$ can be written as

$$\begin{aligned} (\rho_A^i \otimes \rho_B^i)^R &= vec(\rho_A^i) vec(\rho_B^i)^T && (79) \\ &= \left\{(U_A^i)^* \otimes U_A^i \ vec(E_{11}^{m,m})\right\} \left\{(U_B^i)^* \otimes U_B^i \ vec(E_{11}^{n,n})\right\}^T && (80) \\ &= \left\{(U_A^i)^* \otimes U_A^i\right\} vec(E_{11}^{m,m}) vec(E_{11}^{n,n})^T \left\{(U_B^i)^\dagger \otimes (U_B^i)^T\right\}. && (81) \end{aligned}$$

With $vec(E_{11}^{m,m}) vec(E_{11}^{n,n})^T = E_{11}^{m^2,n^2}$ a matrix with the unique singular value 1 is given (the scalars p_i are suppressed during this calculation). As $(U_A^i)^* \otimes U_A^i$ and $(U_B^i)^\dagger \otimes (U_B^i)^T$ are unitary operators, $(\rho_A^i \otimes \rho_B^i)^R$ has the same singular value, namely 1. Therefore the trace norm of the whole state is given by

$$\left\|\rho_{AB}^R\right\|_{\mathrm{Tr}} \leq \sum_i p_i \left\|(\rho_A^i \otimes \rho_B^i)^R\right\|_{\mathrm{Tr}} = \sum_i p_i = 1 \tag{82}$$

In the first step the triangle inequality was used and the desired bound for separable states is obtained, which all entangled states should violate.

As one may has noticed, the realignment criterion is nothing else but distinguishing density operators by calculating their norms in a special way. Therefore another, more analytical approach of proving the realignment criterion shall be mentioned briefly, following the references [38, 39]. This approach starts by defining the so called *cross norm* for the set of trace class operators denoted by $T(\mathcal{H}_A)$ and $T(\mathcal{H}_B)$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$.
An operator T is said to be trace class if

$$\|T\|_1 := Tr(\sqrt{T^*T}) < \infty. \tag{83}$$

Each set $T(\mathcal{H}_A)$ and $T(\mathcal{H}_B)$ can be made to a Banach space by equipping them with the defined trace norm $\| \ \|_1$. Also for composed spaces $T(\mathcal{H}_A) \otimes T(\mathcal{H}_B)$, which are given by the set of all finite linear combinations of composed elements of both sets $\sum_i^n U_i \otimes V_i$, with $U_i \in T(\mathcal{H}_A)$ and $V_i \in T(\mathcal{H}_B)$ $\forall i$, such a norm can be found. By defining the so called *cross norm* as

$$\|T\|_\gamma := \inf \left\{ \sum_i^n \|U_i\|_1 \|V_i\|_1 \ \mid T = \sum_{i=1}^n U_i \otimes V_i \right\}, \tag{84}$$

whereas the infimum is taken over all linear combinations that can be used to define $T \in T(\mathcal{H}_A) \otimes T(\mathcal{H}_B)$ [33], it can be shown [38] furthermore, that if a state $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$ is separable its cross norm has to be smaller or equal 1, $\|\rho\|_\gamma \leq 1$. Also the inverse statement is valid, since from $\|\rho\|_\gamma \leq 1$ the property of ρ being separable can be concluded.
This leads to a Theorem, which is shown to be equivalent to the previously formulated realignment criterion [40]:
An arbitrary bipartite state $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$ is separable, iff $\|\rho\|_\gamma = 1$.

5.2 Permutation criterion

The structure of this criterion is similar to the pt-criterion as it changes the order of the elements of the density matrix (the image (Img) of the matrix) and conducts from it the separability of the original matrix. Also for higher dimensional systems with more particles, i.e. more subsystems, the realignment of matrix-elements permits to give a necessary condition whether a state is separable or not. This generalization of the previous criterion is called the permutation criterion and is defined as follows.
A multipartite state $\rho_{\mathcal{H}_1,\ldots,\mathcal{H}_n}$ with $\mathcal{H}_i$ being of arbitrary dimension is separable, iff the matrix ρ^R with interchanged entries, given by

$$\rho^R := \rho_{\Pi(i_1,j_1,i_2,j_2,\ldots,i_n,j_n)}, \tag{85}$$

holds this inequality:

$$\left\|\rho^R\right\| \leq 1 \tag{86}$$

In this theorem Π denotes the permutation of all indices in the product base. The exact proof or further results of this theorem can be found in references [41, 42].

[33] Actually a crossnorm of a bipartite Banach space is, according to [39], given by $\|T_A \otimes T_B\| = \|T_A\|_1 \|T_B\|_1$, with $T_{A/B} \in T(\mathcal{H}_{A/B})$, whereas the norm $\| \ \|_\gamma$ fulfills this property.

CHAPTER 6

Distillation of Entanglement

Another interesting way of trying to understand entanglement is the so called distillation or purifying of entanglement out of a given bipartite state. The main idea of this method is manipulating the state ρ via the help LOCC operators, i.e. measuring, rotating, phase shifting and ensembles of it. Via this way a new state is created, which carries more entanglement in the sense that it contains more proportions of a certain pure maximally mixed state. The procedure and the sequence, in which the operators are applied to the state is called the *distillation protocol*, which is in this thesis denote as Λ and $\Lambda(\rho)$, respectively.
Such distillation protocols serve the experimental need of regaining maximal entangled singlets out of imperfect noisy quantum channel (noisy entanglement) or mixed states, which are unwanted for certain applications, see for example reference [43].

6.1 Distillation Protocol

Before applying such a distillation protocol onto a state, k copies of it have to be available. In the most general case a mixed state $\rho \in \mathcal{H}^d$ is hence converted to $\rho^{\otimes k} \in H^{d^k}$ and after the protocol has been deployed, these k states are reduced to a certain number m. If assumed that these m remaining states are equal and furthermore "closer" [34] to a maximally or totally entangled state, the protocol is successful. Depending on these two numbers, namely the whole amount of copied states k and the states with successful distillation m, a distillation protocol is said to be optimal if the ratio $\frac{m}{k}$ is maximal for a sufficient large number of copies k. The optimal ratio is denoted as *Distillable Entanglement* E_D [5].
From the mathematical point of view, a distillation protocol Λ is an element of the set $LOCC(\mathcal{H}^d, \mathcal{H}^d)$, mapping operators of one Hilbert space $\mathcal{H}^d$ into itself.

Although there are many ways to construct such a protocol, every Λ can be divided into three different turns, that an arbitrary state ρ has to run through one or several times in order to increase its entanglement.

I Copying the initial state ρ k times: $\rho \to \rho^{\otimes k}$

II Applying certain LOCC operations on $\rho^{\otimes k}$ in order to receive $\rho'^{\otimes m}$ and via projection a new state ρ'

III Comparing the entanglement of the initial state $E(\rho)$ with the one of the new state $E(\rho')$:

- If $E(\rho) \geq E(\rho')$ the protocol failed
- If $E(\rho) < E(\rho')$ the protocol is working properly

If the protocol is working properly the process will be repeated until the entanglement has reached a maximal (i.e. constant) amount, i.e. the entanglement of the state in the previous run is the same as in the actual.

When speaking of *LOCC* operations acting on the k copies of the state ρ (point II), the

[34] Closer means, that the amount of entanglement of the state has increased

most general form of an operation is given by

$$\tilde{\Lambda}(\rho^{\otimes n}) = \frac{\sum_{i=0}^{m} A_i \otimes B_i \otimes ... \otimes S_i \rho^{\otimes k} A_i^\dagger \otimes B_i^\dagger \otimes ... \otimes S_i^\dagger}{Tr(A_i^\dagger A_i \otimes B_i^\dagger B_i \otimes ... \otimes S_i^\dagger S_i)}, \tag{87}$$

with $A_i, B_i, \ldots, S_i$ being unitary operators, acting on the m different subsystems.
The exact definition of an arbitrary bipartite state ρ, that can be successfully distilled, can now be posed [44, 45]:

Definition (distillable state):
Assuming the situation that a bipartite state ρ and a sufficient large number of its copies are shared by two parties, a state or a density operator ρ is said to be distillable if a maximally entangled state can be obtained by allowing both parties only the use of LOCC operations.
Also another an equivalent definition based on distillable entanglement E_D can be given [46]:
A state is called distillable iff the distillable entanglement E_D is strictly larger than zero.

Important representatives of distillation protocols and how their most common operations can increase entanglement is presented in the following:

- First of all a helpful definition is introduced which allows to rewrite a state as a superposition of maximally entangled states.
  Definition (Bell diagonal state) [47]:
  A Bell diagonal state is referred to the two qubit case and defined as mixture of the four Bell states:

$$\rho_{BD} = c_1 \left|\Phi^+\right\rangle\left\langle\Phi^+\right| + c_2 \left|\Phi^-\right\rangle\left\langle\Phi^-\right| + c_3 \left|\Psi^+\right\rangle\left\langle\Psi^+\right| + c_4 \left|\Psi^-\right\rangle\left\langle\Psi^-\right|. \tag{88}$$

  Due to its construction this state has, among other things, the following properties:

  - ρ_{BD} is separable if $c_i \leq 1 \ \forall i \in \{1, 2, 3, 4\}$.
  - In reference [48] it is shown that any bipartite state ρ can be transformed into ρ_{BD} via $\rho_{BD} = \frac{U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger}{Tr(U_A U_A^\dagger \otimes U_B U_B^\dagger)}$, with U_A and U_B being unitary operators on the eligible subsystems.

  The upcoming operations are manipulating the weights c_i and therefore influence the amount of the four Bell states in a arbitrary state. Also for more particles it is possible to distill certain states to more entangled or fully entangled states (chapter 7), however it can not be determined whether a protocol is optimal as no unique generalization of the Bell states exists in the multipartite case (for further results it is referred to chapter 6.2). The following operators are designed to be parts of distillation protocols for the qubit case:

- **Random bilateral rotation:**
  This operation is also called twirling operation and means applying a random element of the SU(2) on both subsystems of a mixed state ρ (written in the Bell basis) in order to receive a rotational symmetric mixture of Bell states,

$$\rho_W = F \left|\Phi^+\right\rangle \left\langle\Phi^+\right| + (1-F)(\left|\Phi^-\right\rangle \left\langle\Phi^-\right| + \left|\Psi^+\right\rangle \left\langle\Psi^+\right| + \left|\Psi^-\right\rangle \left\langle\Psi^-\right|). \tag{89}$$

  These states are called *Werner states* with the *Fidelity* F as a special parameter, $F = \langle\Phi^+| \rho_W |\Phi^+\rangle$, indicating one eligible Bell state. This is shown in [43].

➤ **Unilateral π and bilateral $\frac{\pi}{2}$ rotation:**
Unilateral π operations consist of the Identity and the Pauli operators and are applied on one subsystem of the Bell states:

$$|\Phi\rangle^{\pm} \overset{\sigma_x}{\leftrightarrow} |\Psi\rangle^{+} \quad |\Psi\rangle^{\pm} \overset{\sigma_z}{\leftrightarrow} |\Psi\rangle^{\mp} \quad \Psi^{\pm} \overset{\sigma_z}{\leftrightarrow} \Psi^{\mp} \quad |\Psi\rangle^{\pm} \overset{\sigma_y}{\leftrightarrow} |\Phi\rangle^{\mp} \tag{90}$$

Bilateral $\frac{\pi}{2}$ rotation B_x, B_y, B_z are applied on both subsystems and defined as (overall phases ignored)

$$|\Phi\rangle^{+} \overset{B_x}{\leftrightarrow} |\Psi\rangle^{+} \quad |\Phi\rangle^{-} \overset{B_y}{\leftrightarrow} |\Psi\rangle^{+} \quad |\Phi\rangle^{+} \overset{B_z}{\leftrightarrow} |\Phi\rangle^{-} \tag{91}$$

➤ **Uni- and Bilateral XOR operation:** [35]
The unilateral XOR (UXOR) or CNOT operation was already be mentioned in chapter 2.3. It is defined on a two qubit system, whereas the first qubit is the source and the second one the target qubit. For states written in the computational basis the XOR operation has the following effects:

$$\begin{aligned} |00\rangle &\overset{XOR}{\rightarrow} |00\rangle \qquad |10\rangle \overset{XOR}{\rightarrow} |11\rangle \\ |01\rangle &\overset{XOR}{\rightarrow} |01\rangle \qquad |11\rangle \overset{XOR}{\rightarrow} |10\rangle \end{aligned} \tag{92}$$

The bilateral XOR operation (BXOR) acts on both qubits of the system as well as on its copy. That means that the state has to be copied at least once in order to receive four subsystems, whereas the first of each state are given to Alice, the second two to Bob. Alice and Bob can therefore each define a source and a target system. By combining the two source systems, Alice and Bob receive one of the Bell states (phases omitted) as a combined source system. Proceeding in the same way on the two target systems the effect of the bilateral XOR operation is given as:

Source	Target	BXOR operator	Source	Target
$\Phi^{\pm}$	Φ^{+}	$\longrightarrow$	$\Phi^{\pm}$	Φ^{+}
$\Psi^{\pm}$	Φ^{+}	$\longrightarrow$	$\Psi^{\pm}$	Ψ^{+}
$\Psi^{\pm}$	Ψ^{+}	$\longrightarrow$	$\Psi^{\pm}$	Φ^{+}
$\Phi^{\pm}$	Ψ^{+}	$\longrightarrow$	$\Phi^{\pm}$	Ψ^{+}
$\Phi^{\pm}$	Φ^{-}	$\longrightarrow$	$\Phi^{\mp}$	Φ^{-}
$\Psi^{\pm}$	Φ^{-}	$\longrightarrow$	$\Psi^{\mp}$	Ψ^{-}
$\Psi^{\pm}$	Ψ^{-}	$\longrightarrow$	$\Psi^{\mp}$	Φ^{-}
$\Phi^{\pm}$	Ψ^{-}	$\longrightarrow$	$\Phi^{\mp}$	Ψ^{-}

As already mentioned, the major difference between distillation protocols lies therefore in way, which LOCC operations are used or how they are combined. Herewith a main classification of protocols distinguishes between two different types of protocols. A short sketch of the differences of these two types and how they were introduced in 1996 by Bennett et al. is given in the following. For a more detailed review it is referred to [43]

1. One way hashing distillation protocol

[35] This operation is also known as the C-NOT GATE

This type of protocol allows only a 'one way' communication from a given subsystem to another, not backwards. I.e. informations about measurement results or which operators are used, are only posted from one party, but can be seen from others (the other, in the bipartite case). As this means a restriction of information, it is therefore not possible to distill all states via a one-way procedure. But nevertheless it is useful and sufficient for certain purposes. For more details the reader is referred to the works [49, 50]
The best strategy of the one-way distillation for the bipartite qubit case was introduced in 1996 by Bennett et al. and is called 'hashing'[36]. Again the idea behind this work is, that every state can be written in a mixture of the four maximally entangled bell states $(|\Phi^{\pm}\rangle, |\Psi^{\pm}\rangle)$. In Bennett´s work [49] it is shown that out of a large number of impure pair states k, a smaller number of purified states $l \approx k(1 - S(W))$ can be gained, whenever $S(W) < 1$, with W being the corresponding Werner state. This number of purified states, that are close or even equal to a Bell state, depends beside the number of copies k also on the Entropy [37] of the state [38] $S(W)$, which can be used as a simple entanglement measure in the bipartite case. It is shown further that for k being sufficiently large the ratio $\frac{l}{k}$ yields $1 - S(W)$ and so a lower bound for the distillable entanglement E_D is found: $E_D \geq 1 - S(W)$ [39].

2. Two way distillation protocol

For this class of protocol the restriction of communication is obviously released in such a way that every measurement and operator applied by one party is told to each other by classical communication. Two way protocols are the most commonly used distillation protocols, although they need a lot more copies of the initial state as a one-way protocol. The advantage of allowing full classical communication between the parties lies in the fact, that with the knowledge of all operators and measurement results almost every states becomes distillable [40]. So the two way protocol is the most general form of distillation for bipartite states.
These kind of protocols were also developed by Bennett et al. and just like before his work is followed. In the next lines a special kind of two way protocol, the so called *recurrence protocol*, is introduced:

Alice and Bob start with an arbitrary state, which is again expressed in the Bell basis $(|\Psi^{\pm}\rangle, |\Phi^{\pm}\rangle)$ such that every Bell state vector corresponds to a certain probability p_i:

$$|W\rangle = p_1 \left|\Psi^+\right\rangle + p_2 \left|\Psi^-\right\rangle + p_3 \left|\Phi^+\right\rangle + p_4 \left|\Phi^-\right\rangle \tag{93}$$

When one considers that the protocol favors one certain Bell state, here w.l.o.g. $|\Psi^+\rangle$, it is only the probability p_1 that tells by increasing whether the protocol works and if the state is actually distillable. Therefore one often sees the state written as

$$|W\rangle = F \left|\Psi^+\right\rangle + (1 - F)\left(\left|\Psi^-\right\rangle + \left|\Phi^+\right\rangle + \left|\Phi^-\right\rangle\right) \tag{94}$$

whereas the Fidelity equals p_1 in this case. This Fidelity shows the proportion of a certain maximally mixed singlet into which the initial state will be distilled.
One turn of the protocol is given of the following form:

[36] This term was originally used for quantum cryptography.
[37] The van Neumann Entropy is defined as $S(\rho) = -Tr\left[\rho \log_2(\rho)\right]$.
[38] The state itself is actually an ensemble of Bell diagonal matrices.
[39] Equality is achieved in the case of a original state, that is a mixture of 2 bell states, see reference [5].
[40] That means every Bell diagonal state with eigenvalue greater than $\frac{1}{2}$.

I The initial state ρ expressed in the way as introduced in (93) $\rho_W = \rho_A \otimes \rho_B$ and is copied once $\rho_W^{\otimes 2} = \rho_A \otimes \rho_{\hat{A}} \otimes \rho_B \otimes \rho_{\hat{B}}$, whereas $\rho_{\hat{A}}, \rho_{\hat{B}}$ are the copied subsystems of the eligible parties.
When it comes to applying operations, the systems ρ_A, ρ_B will be called the source system whereas the copied systems $\rho_{\hat{A}}, \rho_{\hat{A}}$ are defined as the target systems.

II Now a bilateral XOR operation on both source as well as on both target systems (Table) is applied, followed by a measurement on the target systems. With the direction of the measurement it is possible to increase the proportion of a particular Bell states, i.e. now it can be chosen whether the protocol favors $|\Psi^{\pm}\rangle$ or $|\Phi^{\pm}\rangle$. If, for instance, the measurement is done in z-direction (assuming the canonical basis) the two states $|\Psi^{\pm}\rangle$ are received, whereas the other two Bell states vanish. As the distillation should only favor one state, here $|\Psi^{+}\rangle$ or $|\Psi^{-}\rangle$, a phase shift or rotation, respectively, can distinguish these two states after the measurement.

III Alice and Bob gain a new state $\rho' = \rho'_A \otimes \rho'_B$ and have to decide whether the protocol was successful or has failed. This is the point when the "two-way protocol " comes into account, since each of the two has to know the results of the measurements performed in the 2nd step. Via classical communication Alice and Bob can split up their initial states into two piles; the one that passed the BXOR operation and the one that failed (Table). In order to see if the distillation worked they compare the changes of the probabilities p_i of the passed states ρ', i.e. nothing else but the different weights of mixtures of bell states:

$$\begin{aligned}
p'_1 &= \frac{p_1^2 + p_2^2}{p_1^2 + p_2^2 + p_3^2 + p_4^2 + 2p_1 2p_2 + 2p_3 2p_4} \\
p'_2 &= \frac{2p_1 p_2}{p_1^2 + p_2^2 + p_3^2 + p_4^2 + 2p_1 2p_2 + 2p_3 2p_4} \\
p'_3 &= \frac{p_3^2 + p_4^2}{p_1^2 + p_2^2 + p_3^2 + p_4^2 + 2p_1 2p_2 + 2p_3 2p_4} \\
p'_4 &= \frac{2p_3 p_4}{p_1^2 + p_2^2 + p_3^2 + p_4^2 + 2p_1 2p_2 + 2p_3 2p_4}
\end{aligned} \tag{95}$$

The denominator represents the probability for the state to pass the bilateral XOR operation.
If the protocol failed ($p'_1 \leq p_1$) and no entanglement was distilled, it can either be the wrong protocol or no entanglement can be distilled out of the state (see next chapter). Otherwise, if $F' = p'_1 > p_1$ the amount of the maximally mixed singlet state $|\Psi\rangle^{+}$ has been increased and the protocol worked. In this case two options are available, which are reconsidered by checking if $E_D = 1 - S(\rho') > 0$, compare reference [13]:

- If indeed $1 - S(\rho') > 0$, the one way protocol works and it is possible to continue the distillation of ρ' by only allowing a restricted communication.
- Independent from the distilled entanglement E_D an iteration of the two-way protocol is always possible as long as the Fidelity F increases every turn. It has to be noted that after each turn the new state has to undergo a twirl operation (random bilateral rotation) in order to start again with a Werner state.

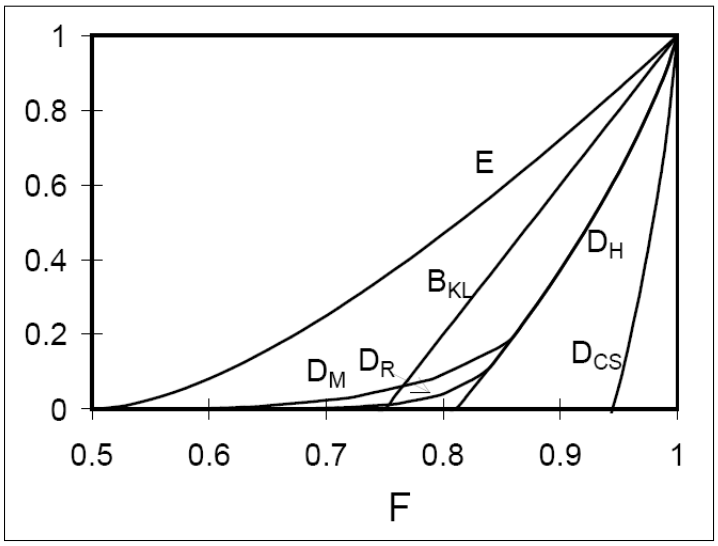


Figure 6: Entanglement over Fidelity of Werner states from [49]

In Figure 6 different types of protocols and different sequences of one way and two way protocols, respectively, are shown by plotting the amount of entanglement, which is determined by certain measures (chapter 7), over the Fidelity of the Werner state. The graphic shows that for states with $F \leq \frac{1}{2}$ no entanglement is distillable ($E_D = 0$), neither with two way protocols nor with one way. Hence two way protocols work for $F > \frac{1}{2}$, whereas one-way protocols even require a Fidelity larger then 0.801 (see reference [43]). The D_H line for example is the result of a one way hashing protocol, which was used to continue two possible two way protocols D_M and D_R. The E line is received by the Entanglement of Formation, which will be defined and explained in chapter 7.

6.2 Multipartite Distillation

The task of distilling entanglement is quite clear when talking about two qubits. Also for the generalized bipartite case with an arbitrary degree of freedom on each subsystem, distillation may be possible, since the maximally entangled states are uniquely defined as well as the Pauli operators can be replaced by Weyl- or Gellman operators. However, as already seen in the previous chapters, the problem in the multiparticle case already arises in the generalization of the Bell states as maximally entangled singlets. The entanglement, which is carried by generalized GHZ or W states differs completely from the qubit case. So it still remains open whether the distillation shall favor one of these totally entangled states, a maximally entangled bipartite cut of a multipartite system or again a Bell state singlet as in the original protocols.
Regarding distillation of multipartite qubit systems the possible approach of taking a GHZ or W state as the favored aim state has already been considered. This chapter shows in detail how such a protocol is constructed and how it differs from previous constructions by using the maximally entangled tripartite W state as the target state, that has to be distilled [51]. The main idea of a successful protocol is introducing the W-Base, that comprises in the tripartite case the following eight vectors $|W_{k_1k_2k_3}\rangle$. It is obtained by applying the unitary operator $U_W := \frac{1}{\sqrt{3}}\mathbb{1}^A\sigma_X^B\sigma_X^C + \sigma_Z^A\sigma_X^B\mathbb{1}^C + \sigma_X^A\mathbb{1}^B\sigma_X^C$ on the eligible standard basis vector $|k_1k_2k_3\rangle$, $k_i \in \{0,1\}$.

$$|W_{k_1k_2k_3}\rangle := U_W\,|k_1k_2k_3\rangle \tag{96}$$

The complete base is hence given as

$k_1k_2k_3$	$\|W_{k_1k_2k_3}\rangle$	$k_1k_2k_3$	$\|W_{k_1k_2k_3}\rangle$
000	$\frac{1}{\sqrt{3}}(\|001\rangle + \|010\rangle + \|100\rangle)$	100	$\frac{1}{\sqrt{3}}(\|101\rangle - \|110\rangle + \|000\rangle)$
001	$\frac{1}{\sqrt{3}}(\|000\rangle + \|011\rangle - \|101\rangle)$	101	$\frac{1}{\sqrt{3}}(\|100\rangle - \|111\rangle - \|001\rangle)$
010	$\frac{1}{\sqrt{3}}(-\|011\rangle + \|000\rangle + \|110\rangle)$	110	$\frac{1}{\sqrt{3}}(-\|111\rangle - \|100\rangle + \|010\rangle)$
011	$\frac{1}{\sqrt{3}}(-\|010\rangle + \|001\rangle - \|111\rangle)$	111	$\frac{1}{\sqrt{3}}(-\|110\rangle - \|101\rangle - \|011\rangle)$

Corresponding to these W base a special set of 8 stabilizers K_j can be constructed by the combination of Pauli operators with respect to the stabilizer condition $K_j \left|W\right\rangle_{k_1k_2k_3} = (\pm 1)^{k_j} \left|W\right\rangle_{k_1k_2k_3}$ (chapter 2.3). The first three are given by

$$\begin{aligned}
K_1 &= \frac{1}{3}\big[2(\sigma_X \otimes \sigma_X \otimes \sigma_Z) + 2(\sigma_Y \otimes \sigma_Z \otimes \sigma_Y) + 2(\sigma_Z \otimes \mathbb{1} \otimes \mathbb{1})\big], \\
K_2 &= \frac{1}{3}\big[2(\sigma_Z \otimes \sigma_X \otimes \sigma_X) + 2(\sigma_Y \otimes \sigma_Y \otimes \sigma_Z) + 2(\sigma_Z \otimes \mathbb{1} \otimes \mathbb{1})\big], \\
K_3 &= \frac{1}{3}\big[2(\sigma_X \otimes \sigma_Z \otimes \sigma_X) + 2(\sigma_Z \otimes \sigma_Y \otimes \sigma_Y) + 2(\mathbb{1} \otimes \mathbb{1} \otimes \sigma_Z)\big],
\end{aligned}$$

whereas the other 5 are given by their combinations. Therefore the set of stabilizers is given by $\{\mathbb{1}, K_1, K_2, K_3, K_1K_2, K_1K_3, K_2K_3, K_1K_2K_3\}$. Now the actual protocol $\mathcal{P}$ can be applied. W.l.o.g. it is assumed that $\left|W_{000}\right\rangle \left\langle W_{000}\right|$ is the greatest proportion of the state to be distilled. Hence it can be written in a way that $\rho = F \left|W_{000}\right\rangle \left\langle W_{000}\right| + (F-1) \left|\text{noise}\right\rangle$. Mathematically the protocol $\mathcal{P}$ turns three copies of the state ρ (i.e. $\rho^{\otimes 3}$) into a state ρ' by

$$\rho' = \sum_{m=1,2,3} PM_m^{(A)} PM_m^{(B)} PM_m^{(C)} \rho^{\otimes 3} M_m^{(A)\dagger} PM_m^{(B)\dagger} PM_m^{(C)P\dagger}, \tag{97}$$

with

$$M_{m^{(l)}}^{(l)} = \frac{1}{4}\big(\mathbb{1} + (-1)^{m_1^{(l)}} K_1^{(l)} K_2^{(l)}\big)\big(\mathbb{1} + (-1)^{m_2^{(l)}} K_1^{(l)} K_3^{(l)}\big), \tag{98}$$

whereas $l \in \{A, B, C\}$ and the completeness relation $\sum_{m^{(l)}} M_{m^{(l)}}^{(l)\dagger} M_{m^{(l)}}^{(l)} = 1$ holds. The operator P is a special projector, mapping the three copies of ρ into a single copy of the state, with regards to the index $m^{(l)}$ or also denoted as m (if the subsystem is obvious), which again corresponds to the result of $M_{m^{(l)}}^{(l)} \rho^{\otimes 3} M_{m^{(l)}}^{(l)\dagger}$. Since there are three subsystems each controlling three qubits after the state ρ is copied and $M_{m^{(l)}}^{(l)}$ comprising the two stabilizers $K_1^{(l)}K_2^{(l)}$ and $K_1^{(l)}K_3^{(l)}$, two out of the three qubits give its eigenvalues as the result of this operation. Hence m is assigned to these three different outcomes $[0,1] := 1 \mathrel{\hat{=}} m_1^{(l)}$,$[1,0] := 2 \mathrel{\hat{=}} m_2^{(l)}$ and $[0,1] := 3 \mathrel{\hat{=}} m_3^{(l)}$. After comparing these outcomes, the three subsystems arrange to choose the same projection operator P on the same outcomes (in the following denoted by $P_i^{(l)}$), i.e. if $m = 1$ the operator $P_1^{(l)} : \left|W_{000}\right\rangle^{(l)} \to \left|0\right\rangle^{(l)}, \left|W_{110}\right\rangle^{(l)} \to \left|1\right\rangle^{(l)}$ reduces the three qubits of a subsystem to one qubit, if $m = 2$, $P_2^{(l)} : \left|W_{010}\right\rangle^{(l)} \to \left|0\right\rangle^{(l)}, \left|W_{101}\right\rangle^{(l)} \to \left|1\right\rangle^{(l)}$ or for $m = 3$, $P_3^{(l)} : \left|W_{100}\right\rangle^{(l)} \to \left|0\right\rangle^{(l)}, \left|W_{011}\right\rangle^{(l)} \to \left|1\right\rangle^{(l)}$.
Depending on the kind of noise a state is polluted with or how much noise is added, respectively, this protocol can completely distill the W state by iteration of this method. For a

state with an arbitrary noise however, this protocol has to be extended. But before doing so, it may be helpful to stress the physical logic behind this protocol:

- The state ρ is rewritten in the W-basis and copied three times such that every party A,B and C receives three qubit on which they can perform the defined local measurements.
- The local measurements are given by the combination of particular stabilizer operators for the W basis K_1K_2, K_1K_3. They are applied on two of the three qubits on each subsystem A,B and C.
- The corresponding outcome of each party is the 2 bit value $m^{(l)} = [m_1, m_2]$, with $l \in \{A, B, C\}$. The value $m^{(l)}$ can yield three different results, which are shared by each party (That means, that this protocol is a two-way distillation protocol). If all three outcomes $m^{(l)}$ are equal each party performs the above defined projector P corresponding to one of the three $m^{(l)}$.
- If the outcomes $m^{(l)}$ do not coincide, the measurement is discarded and the process is repeated. Otherwise a new state ρ' is received, containing more properties of the $|W_{000}\rangle$ state, hence the Fidelity F is increased. Normalizing and repeating this process may increase the Fidelity further

When dealing with an arbitrary noise, the protocol is extended by its dual protocol $\bar{\mathcal{P}}$. Although the operators are defined slightly different, the structure of the previous points are the same. The stabilizers are changed by a combination of the Hadamard operator, here defined for each party A,B,C (superindex (l)) and within each party for the three qubits 1,2,3 (subindex i) $H_i^{(l)} := \frac{1}{\sqrt{2}}(\sigma_X + \sigma_Z)$, and the swap operator $\text{swap}_{ij} : |kk'\rangle \to |k'k\rangle$, with $k, k' \in \{0, 1\}$ switching the i-th with the j-th element of the tensor product. Hence the complementary stabilizers are given by $\bar{K}_j^{(l)} = \Lambda^{l\dagger} K_j^{(l)} \Lambda l$, with $\Lambda^l = H_1^l H_2^l H_3^l \text{swap}_{13}^l$. These stabilizers are combined in the same way as in the previous protocol, but the fundamental change, due to this new definition, is that the measurement is realized in a complementary base. Therefore the preparation of the state ρ is not only done by copying it three times but also by transforming the computational basis into the complementary base. This is obtained with an operator V exchanging the vectors in the way that $|000\rangle \leftrightarrow |000\rangle, |111\rangle \leftrightarrow |111\rangle, |100\rangle \leftrightarrow |011\rangle, |010\rangle \leftrightarrow |101\rangle$ and $|001\rangle \leftrightarrow |110\rangle$. Therefore after the state is prepared as $V^A V^B V^C \rho^{\otimes 3} V^{A\dagger} V^{B\dagger} V^{C\dagger}$, the distillation follows the same procedure using the complementary operators. However for this dual protocol $\bar{\mathcal{P}}$ the only measurement outcome in which the three subsystem can coincide is given by $m = [0, 0]$. This leads to the fact that only one projector has to be defined that reduces the three qubits of each party to one: $\bar{P}_0^l : |\bar{W}_{000}\rangle \to H |1\rangle^l, |\bar{W}_{111}\rangle \to H |0\rangle^l$

Which of the two protocols $\mathcal{P}$ or $\bar{\mathcal{P}}$ can actually increase the W-state proportion is a priori unclear, unless by complete state tomography, i.e. determine each of the entries of the density matrix of the initial state. Another drawback of this protocol is the uncertainty of the final state, that differs between three different outcomes. This drawback turns out to be a fascinating effect, as, for an arbitrary density matrix, the Fidelity is the main factor indicating which way this recurrence protocol takes.

- If the fidelity is about 0.7, the W-state will be predominated, as more than 99 per cent of the initial states can be distilled

- If the fidelity drops under 0.7, the outcome will be unclear as the protocol favors either the W-state or a two qubit Bell state that is shared by two of the three subsystems, e.g. $\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\,|0\rangle$ or a undistillable state

This effect is quite surprising as the Bell state is not part of the states who are eigenstates of the used stabilizers.

6.3 Bound entanglement

The success of distillation protocols grew further as one could show in [52] that every two qubit state, which is entangled, can be distilled. But against previous assumptions, that this is also true for every bipartite state with higher dimensions, it turned out that there exist states (already for $\mathcal{H}^3 \otimes \mathcal{H}^3$), which are entangled but can not be distilled [53]. For these special entangled states there is a need for a new definition, stated for example in [5, 46]:

Definition (bound entangled state):
A state ρ is called bound entangled iff no maximally entangled state can be distilled out of it.

As there exist infinite ways of distillations it is hard to say whether a given state is bound entangled or not.

This phenomena of entanglement was discovered comparatively late, since it occurs only in states with $\mathcal{H}^a \otimes \mathcal{H}^b > 6$.

Reminding the partial transposition criterion, one notices a similarity in the spaces where the pt-condition is sufficient and necessary. It is not surprising, that an entangled state with positive partial transposition is bound entangled. And indeed a connection between distillation and partial transposition was found, which is, until today, not fully understood, and will be discussed in the next section.

6.4 Beyond Distillation

This obviously new kind of entanglement, which is found in bound entangled states, is one of the major tasks in the study of quantum entanglement as it is until now an open question how such states can be constructed or even distinguished.
Every notified bound entangled state is revealed as a PPT state, when the Peres criterion is applied. So the question arises whether bound entanglement is only possible within the set of PPT states?
In 1998 the Horodeckis came up with a promising theorem, that opened an approach to this question formulated in [54]:

Theorem:
A bipartite state ρ on $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$ is distillable iff there exist two projectors $P : \mathcal{H}_a^{\otimes k} \to \mathcal{H}^2$ and $Q : \mathcal{H}_b^{\otimes k} \to \mathcal{H}^2$ such that for some $k \geq 1$ the state

$$\rho' = (P \otimes Q)\rho^{\otimes k}(P \otimes Q)^\dagger \tag{99}$$

is entangled.
Since the resulting state acts on $\mathcal{H}^2 \otimes \mathcal{H}^2$ Hilbert space, this is equivalent to a negative partial transposition of ρ
Corresponding to this theorem, a useful definition was introduced:

Definition (pseudo k copy distillable or k-distillable):
A bipartite as well as a multipartite state ρ is called *pseudo k copy distillable*, or shorter *k-distillable*, if the condition of this theorem is fulfilled for a certain number of copies k.
With this definition the number of required copies is described in order to gain a successful protocol.

In the following a few promising partial results founding on the above theorem are collected:

- In [55] it is shown that all qubit states of dimension $\mathcal{H}^2 \otimes \mathcal{H}^k$ are distillable iff they are NPT states.
  For achieving this result much groundwork was done by Horodecki et al. [52], when they showed that every bipartite state is distillable iff it is entangled.
- Every NPT state can be transformed into an NPT Werner state using LOCC operations. Therefore the question whether there is a NPT bound entangled state can be reduced to the question whether there exist NPT bound entangled Werner states, as claimed in reference [56].
- According to reference [57], the property of a state whether it is distillable or not can be shifted into a Schmidt number problem. The crucial idea behind this follows from the previous Theorem.
- If the the rules of distillation are changed by allowing beside LOCC also PPT preserving operations, all NPT states can be distilled with a single copy of the NPT state, as shown in reference [58]. This result is shown by using separable superoperators S, which are an equivalent formulation of the two way communication protocol, since it can be shown that a state can be distilled, iff $Tr\left[P_m S(\rho)\right] > \frac{1}{m}$ with $P_m = |\Psi_m\rangle\langle\Psi_m|$ being the projector onto the maximally entangled state in $m \times m$ dimensions. Furthermore a separable superoperator is a completely positive, trace preserving linear transformation, whose explicit definition can be found in reference [59]

CHAPTER 7

Entanglement measures

This chapter is dealing with the one of the most fundamental question since entangled states were discovered. Soon after the development of quantum entanglement the search for a sufficiently simple measure with suitable properties began and has not ended yet. But why is quantifying entanglement and finding a good measure such a hard task? In the following chapter this question will be tackled by introducing different approaches as well as different types of entanglement measures. The main goal is defining a measure that fits best in order to deal with upcoming results of describing quantum systems in a geometrical way.

7.1 Basics about measures

When speaking about measures in a general mathematical way one thinks of a linear functional E, that maps elements of one vector space or a Hilbert space, respectively, into $\mathbb{C}$ or more general the underlying scalar body. Furthermore a few axioms have to be proposed in order to receive a measure. These axioms have to be fitted on this special purpose, namely quantifying entanglement, and therefore they differ from the mathematical point of view. In the following the most commonly used axioms for entanglement measures are introduced, whereas not all of them have to be fulfilled in order to be a proper measure. Another approach in quantifying entanglement via state manipulation is shortly sketched after introducing the most import axioms, that are also found in [6, 9] for instance.

- *Positivity:* $E(\rho) \geq 0$
  This has to be fulfilled for all $\rho \in \mathcal{H}$. But this axiom is rather a technical, mathematical axiom and can easily achieved by shifting, as the measure was mentioned to be linear.

- *Normalization:* $E(\rho) = 0$ iff $\rho = 0$
  For an entanglement measure this property has to be expanded in such a way that $E(\rho) = 0 \quad \text{iff} \quad \rho \in SEP$. Along with the normalization another (optional) property for a measure is often demanded when it is applied on a maximally entangled bipartite state, e.g. $|\Psi\rangle$: $E(|\Psi\rangle^{\otimes n}) = n$ (compare additivity axiom). For higher dimensions this property can not be claimed, as there is no unique definition of a maximally entangled states.

- *Non increasing under LOCC:* $E(\Lambda(\rho)) \leq E(\rho)$
  Λ is chosen from the set of positive maps that is uniquely referred to the set of LOCC operations, as it is shown in the second chapter.
  Following reference [9] also the description with Kraus operators K_i instead of positive maps is possible:

$$\sum_i p_i \; E\Big(\frac{K_i \rho K_i^\dagger}{Tr(K_i \rho K_i^\dagger)}\Big) \leq E(\rho) \quad \text{with } p_i = Tr(K_i \rho K_i^\dagger) \tag{100}$$

  As a more specific version of this condition it is often demanded that the measure does not increase under LOCC operations on average. This means that assuming a LOCC map, which maps a state ρ with probability p_k to a state ρ_k the inequality

$$\sum_k p_k \; E(\rho_k) \leq E(\rho) \tag{101}$$

holds.

- *Unitary invariance:* $E(\rho) = E(U\rho U^\dagger)$
  The amount of entanglement of state should also be invariant under unitary transformations.

- *Convexity:* $E(\sum_i p_i\ \rho_i) \leq \sum_i p_i\ E(\rho_i)$
  The convexity tells about the behavior of the measure, when it is applied locally. One sees that the entanglement of a state reaches a maximal value when the entanglement of every subsystem is determined separately and summed up. That also means that the more information is known about the subsystems, the higher amount of entanglement is detected. Although this axiom is a necessary one from a mathematical point of view, it can not be fulfilled by some entanglement measures.

- *Additivity Properties:*
  Considering n different states ρ_i with $i = 1, 2, ..., n$, which are mutual independent from each other. The entanglement measured in the composed Hilbert space, comprising all systems, should yield the same amount as adding up the amount of entanglement of the states measured in their individual Hilbert spaces:

$$E(\rho) = E(\rho_i \otimes \rho_j \otimes ... \otimes \rho_n) = E(\rho_i) + E(\rho_j) + ... + E(\rho_n) \tag{102}$$

  Contrary to the convexity, it has to be noted that this equality is addressed to n independent quantum systems with no interaction. Also a weaker additivity condition exists, which is a special case of the previous one, as one state ρ is copied n times:

$$E(\rho) = E(\rho \otimes \rho \otimes ... \otimes \rho) = E(\rho^{\otimes n}) = nE(\rho) \tag{103}$$

These requirements are not obeyed by all entanglement measures and can be seen as optional, but self-evident and useful. A function $E(\rho)$ that fulfills the first three points plus the convexity axiom is called *entanglement monotone* and can be seen as the pre-stage of a measure (see reference [9]).

7.2 Entanglement of Formation

The construction of an entanglement measure can be realized, as already mentioned, in various ways. Beside introducing the stated conditions the already known distillable Entanglement E_D (chapter 6) can also serve as a measure. Distillation of entanglement was developed in order to determine how many maximally entangled states (m) can be produced out of a given state ρ by copying and applying only trace preserving LOCC operations $\Lambda(\rho^{\otimes n})$. This means in a precise mathematically way that the ratio E_D $(= \frac{m}{n})$ can be found when the difference between a distilled bipartite state ρ and a certain number of maximally entangled bipartite state $\left|\Psi_d^+\right\rangle\left\langle\Psi_d^+\right|$ vanishes,

$$E_D(\rho) := \sup\left\{r \mid \lim_{n\to\infty}\left[\inf_{\Lambda} Tr(\Lambda(\rho^{\otimes n}) - \left|\Psi_d^+\right\rangle\left\langle\Psi_d^+\right|^{\otimes rn})\right] = 0\right\}. \tag{104}$$

Also the consideration from the other direction, namely how many maximally entangled states are necessary in order to rebuild a given state ρ by using trace preserving LOCC operations, leads to a commonly used entanglement measure, which is called *entanglement cost* and defined as

$$E_C(\rho) := \inf\left\{r \mid \lim_{n\to\infty}\left[\inf_{\Lambda} D(\rho^{\otimes n}, \Lambda(\left|\Psi_d^+\right\rangle\left\langle\Psi_d^+\right|^{\otimes rn}))\right] = 0\right\}, \tag{105}$$

with the difference, that in this case the measure of entanglement is shifted to a measure of distance between two states ρ and σ, denoted by the functional $D(\rho, \sigma)$, found in reference [60].
As E_D and E_C have the same underlaying structure, it is not surprising that for bipartite pure state $E_D(\rho) = E_C(\rho) = S(Tr_A(\rho)) = S(Tr_B(\rho))$, with $S(\rho) = -Tr(\rho \log_2(\rho))$ being the so called *von Neumann entropy*. Furthermore basing on the this result for pure states a measure for arbitrary states ρ can be constructed via the so called *Entanglement of Formation* E_F [49, 9],

$$E_F(\rho) = \inf_{p_i, |\Psi_i\rangle} \Big\{ \sum_i p_i S\left[Tr_B(|\Psi_i\rangle \langle\Psi_i|)\right] \ : \ \rho = \sum_i p_i \ |\Psi_i\rangle \langle\Psi_i| \Big\}. \tag{106}$$

It can be shown [61] that in the asymptotic limit of infinite copies ($n \to \infty$) E_F and E_C are equal $\lim_{n\to\infty} \frac{E_F(\rho^{\otimes n})}{n} = E_C$. With this construction the problem of the entanglement measure for a mixed state is returned to a convex superposition of pure states, that represents the mixed state. Such a construction is called *convex roof* and is, as there is no unique decomposition of a mixed state, in general hard to calculate analytically. The loophole out of this drawback are bounds that can approximate the infimum of this decomposition. The advantage of convex roof measures are its properties, which are directly taken over from the pure state case, such as convexity, positivity or non increasing under LOCC.

Concurrence:
The concurrence, or Wootter´s and Hill Concurrence [62, 63], is an elegant way of analytically calculating E_F for an arbitrary bipartite qubit state. The secret behind this is a certain expression of the entropy function for pure states, namely the binary entropy function

$$H(x) = -\left[x \log_2 x + (1-x) \log_2 (1-x)\right], \quad \text{with } 0 \leq x \leq 1, \tag{107}$$

and therefore also for the amount of entanglement of a pure state $\epsilon(x) = H(\frac{1}{2} + \frac{1}{2}\sqrt{1-x^2})$ [41]. Combined with a special basis, the Bell-basis with particular phases $\{e_i, i = 1, ..., 4\}$, in which any pure state can be written as $|\Psi\rangle = \sum_i \alpha_i |e_i\rangle$, its entanglement can be expressed in terms of its coefficients α_i

$$E_F(|\Psi\rangle) = \epsilon(\Big|\sum_i \alpha_i\Big|). \tag{108}$$

The argument of the function ϵ, here $|\sum_i \alpha_i|$, is called concurrence. The concurrence itself must be seen as a function of the state, $C(|\Psi\rangle)$, which already acts as some kind of measure as it ranges from 0 to 1 and its monotonicity is connected to E_F. Therefore this formula is often written in the more general way, using the concurrence function $C(|\Psi\rangle)$,

$$E_F(|\Psi\rangle) = \epsilon(C(|\Psi\rangle)). \tag{109}$$

The generalization of this construction to arbitrary states ρ is done by defining the following operator valued functional $R(\rho)$,

$$R(\rho) = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}, \tag{110}$$

[41] The argument of H is chosen in this way to make sure that the values of the resulting entanglement measure lies in between 0 and 1.

that replaces $E(|\Psi\rangle)$. Here $\tilde{\rho}$ is the complex conjugated of ρ, which is given by the previously introduced basis vectors $\{e_i, i = 1, ..., 4\}$ [42]. With this knowledge the following Theorem can be posed:

Theorem:

For ρ being a density matrix of a two qubit system, with two eigenvalues unequal to 0, the Entanglement of Formation is given by

$$E_F(\rho) = \epsilon(C(\rho)) \quad \text{with} \quad C(\rho) = \max\{0, 2\lambda_{\max}(\rho) - Tr[R(\rho)]\}. \tag{111}$$

R was explained before and $\lambda_{\max}$ is the largest eigenvalue of R.

The proof of this theorem can be found in reference [62].

This theorem could be generalized further using the so called *spin flip transformation* [63]. For a pure state $|\Psi\rangle$ the spin flipped state, here denoted with the tilde symbol, is defined as

$$\left|\tilde{\Psi}\right\rangle = \sigma_y |\Psi\rangle^*. \tag{112}$$

With this definition the concurrence for pure states can be alternatively expressed by $C(|\Psi\rangle) = \left|\left\langle \Psi, \tilde{\Psi} \right\rangle\right|$.

This spin flip transformation is generalized to an arbitrary state ρ by taking the complex conjugation in exactly the above mentioned basis $\{e_i, i = 1, ..., 4\}$. Hence the the functional R can be expressed as

$$R(\rho) = \sqrt{\sqrt{\rho}(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)\sqrt{\rho}} \tag{113}$$

with ρ^* now given in the standard base.

The entanglement of formation E_F can hence be formulated with this generalized concurrence:

For a quantum state ρ, describing a two qubit system, the E_F is given by

$$E_F(\rho) = \epsilon(C(\rho)) \quad \text{with} \quad C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} \tag{114}$$

whereas the λ_i are the eigenvalues of the Hermitian matrix $R(\rho)$ in decreasing order or, as an equivalent definition, the λ_i´s are the square roots of the non Hermitian matrix $\rho\tilde{\rho}$. For a pure state, $R(\rho_{pure})$ has only one non-zero eigenvalue.

Although one can expand this result to higher dimensions (concurrence vector, see reference [64]) the optimization over all pure states remains inevitable for higher dimensions. A nice attempt of generalizing this result to a multidimensional measure is introduced in the following and will be applied to illustrate the geometry of states.

7.3 Multipartite Entanglement Measures

In order to receive a multipartite measure and generalize the previous construction one possible and promising way is the enhancement of the introduced flip operator (111) and (112), respectively. As this measure should work for an arbitrary amount of particles with arbitrary degrees of freedom, it has to distinguish between the different types of entanglement, i.e. between which subsystem or between which groups of subsystems the entanglement can be found (k-separability).

Therefore a useful way of looking at a quantum system is regarding the partition of the information content by using an equation related to Bohr´s complementary condition, known

[42] $R(\rho)$ also ranges from 0 to 1 and can be understood as a kind of measure of the equality between ρ and $\tilde{\rho}$ as it is invariant under local unitary transformation.

for example from the double slit [65]. For an n partite system the equation

$$I(\rho) + R(\rho) + E(\rho) = n \tag{115}$$

can be proposed. With the three functions $I(\rho)$, $E(\rho)$ and $R(\rho)$:

- $I(\rho)$ contains all locally obtainable information of the quantum system and comprises all subsystems, $I(\rho) = \sum_{s=1}^{n} S_s^2(\rho)$.
- $E(\rho)$ denotes the information content bounded in entanglement between all subsystems
- $R(\rho)$ is the remaining unavailable information traced to the uncertainty of the measurement result of the quantum state itself.

It remains to explain the quantity $S(\rho)$, that is summed up in order to obtain $I(\rho)$, which is explained in the first point. Formerly introduced to describe the theoretical information content of the double slit experiment, the original complementary relation by Bohr,

$$S^2(\rho) := P^2(\rho) + C_{coh}^2(\rho) \leq 1, \tag{116}$$

can be adapted to an arbitrary two state quantum system. $C_{coh}(\rho)$ and $P(\rho)$ are known as the *visibility* [43] and *predictability* [44], respectively, or more general, $C_{coh}(\rho)$, the coherence and, $P(\rho)$, the a priori knowledge of the state. The complementary relation turns out to be an equality as long as pure states are described, otherwise it is possible to restore the equation out of the inequality by adding a function $M(\rho)$, which can be seen as a measure of the mixedness, the classical uncertainty of the quantum state. It is defined by $M^2(\rho) := \frac{d}{d-1}[1 - Tr(\rho^2)]$. Herewith the complementary relation yields

$$S^2(\rho) + M^2(\rho) = 1. \tag{117}$$

The next step in constructing a multipartite "concurrence-like " measure is finding a similar expression to the latter one (110) for higher dimensions. In reference [65] this problem is solved by writing the probability for a certain qudit state ρ as

$$P_g^2(\rho) = \frac{d-1}{d} \sum_{\pi} \left| P_{0,0} - \frac{P_{1,1} + P_{2,2} + ... + P_{d-1,d-1}}{d-1} \right|^2 . \tag{118}$$

$\sum_{\pi}$ denotes the sum over all possible permutations of $P_{i,i}$. When considering again the above used analogy of an interference pattern, one permutation describes the probability of the particle taking a certain path minus the probabilities of the remaining paths. Using the completeness relation of the probabilities $P_{i,j} := Tr(\rho \left|i\right\rangle \left\langle j\right|)$, $\sum_i P_{i,i} = 1$, this quantity reduces to

$$P_g^2(\rho) := \frac{d}{d-1} \sum_{i} \left| P_{i,i} - \frac{1}{d} \right|^2 = \frac{d}{d-1} \sum_{i} P_{i,i}^2 - \frac{1}{d-1}. \tag{119}$$

A similar generalization of the coherence again with the quantity $P_{i,j}$, brings the formula

$$C_{coh,g}^2(\rho) := \frac{2d}{d-1} \sum_{j=1}^{d-1} \sum_{i<j} |P_{i,j}|^2 = \frac{d}{d-1}(Tr(\rho^2) - \sum_{i} P_{i,i}^2) \tag{120}$$

[43] Here the visibility of the interference pattern is denoted, which is connected with the wave property a particle.
[44] The predictability denotes the probability of the way, which the eligible particle will take.

The right side is obtained by $Tr(\rho^2) = \sum_{i<j} |P_{i,j}|^2 = \sum_i P_{i,i}^2 + 2\sum_{i,j,i<j} |P_{i,j}|^2$ [45].

Verifying Bohr´s complementary relation by summing up the generalized quantities, $P_g^2(\rho) + C_{coh,g}^2(\rho) = \frac{d}{d-1} Tr(\rho^2) - \frac{d}{d-1} = M^2(\rho) + 1$ yields

$$P_g^2(\rho) + C_{coh,g}^2(\rho) + M^2(\rho) = 1. \tag{121}$$

Based on this equation, an entanglement measure for multipartite quantum systems and a generalized concurrence, respectively, can be introduced: As mentioned before, M can be used as a measure itself, because it fulfills the required axioms [66], and the amount of entanglement of a pure state is herewith given by

$$E(|\Psi\rangle) := \sum_{s=1}^{n} M^2(\rho_s), \tag{122}$$

with ρ_s being the reduced density matrix of $|\Psi\rangle$ to the subsystem s,
$\rho_s = Tr_{[1,...,s-1,s+1,...,n]}(|\Psi\rangle\langle\Psi|)$. The functional $M(\rho)$ is now chosen as the linear Entropy ($S_L(\rho) := 1 - Tr(\rho)$), with the advantage of an easier calculable functional compared to other possible choices, e.g. the von Neuman Entropy. This advantage of the linear entropy is the fact, that it can be expressed in terms of operators, i.e. modified Gellmann operators, that are applied on the density matrix of the pure state to be measured. They are defined as

$$\sigma_{kl}^{d\times d} |k\rangle = |l\rangle, \quad \sigma_{kl}^{d\times d} |l\rangle = |k\rangle, \quad \sigma_{kl}^{d\times d} |t\rangle = 0 \quad \forall t \neq k, l, \tag{123}$$

with $k, l \in \{0, 1, ..., d-1\}$. For a qubit system the flip operation is achieved by the σ_x matrix (compare Wootter´s and Hill´s concurrence)

$$\widehat{O}_{\{\alpha_j\}} := (\sigma_{k_i,l_i}^{s\in\{\alpha_j\}}, \mathbb{1}^{s\neq\{\alpha_j\}}), \tag{124}$$

where the set $\{\alpha_j\} := \alpha_1, \alpha_2, ..., \alpha_m$ [46] indicates the subsystems α_i, on which a flip operator is applied. Because this construction is generalizing the previously introduced concurrence measure, the so-called m-concurrence can be posed. The value m denotes the number of flip operations that are applied on the subsystems. E.g. the 2-flip concurrence is calculated by flipping two subsystems and yields the entanglement between two subsystems. That means that for $m = 2$ this construction is equivalent to the Wootter´s and Hill´s concurrence.

$$E(\rho) = \underbrace{E_{(2)}}_{\text{bipartite entanglement}} + \underbrace{E_{(3)}}_{\text{tripartite entanglement}} + \ ... \ + \underbrace{E_{(n)}}_{\text{n-partite entanglement}}. \tag{125}$$

with the substructure

$$\begin{aligned} E_{(2)} &= E_{(12)} + E_{(13)} + ... + E_{(1n)} + ... + E_{(nn)} \\ E_{(3)} &= E_{(123)} + E_{(124)} + ... + E_{(12n)} + ... + E_{(nnn)} \\ &\vdots \\ E_{(n)} &= E_{(12...n)} \end{aligned} \tag{126}$$

whereas $E_{(ij...k)}$ is the entanglement between the i-th, j-th, ..., k-th subsystem. Expressed with the m-concurrence the entanglement is given by

$$E(\rho) := \underbrace{C_{(2)}^2(\rho)}_{\text{two flip concurrence}} + \underbrace{C_{(3)}^2(\rho)}_{\text{three flip concurrence}} + \ ... \ + \underbrace{C_{(n)}^2(\rho)}_{\text{n-flip concurrence}} \tag{127}$$

[45] $\rho^\dagger = \rho$, $Tr(\rho^2) = 1 = \sum_{i<j} |P_{i,j}|^2$ and the completeness relation is used.
[46] They are defined in decreasing order, $\alpha_1 < \alpha_2 < ... < \alpha_m$, to avoid multiple counting.

In order to get all different amounts of entanglement $E_{(m)}$, one summand $C^2_{(m)}$ has to comprise all combination of subsystems ($\{\alpha_j\}$) [47]:

$$C^2_{(m)} = \sum_{\{\alpha_j\}} C^2_{\{\alpha_j\}}. \tag{128}$$

The concurrence itself is defined via the flip operator:

$$C^2_{\{\alpha_j\}} := \sum_{set} \left| \left\langle \Psi \left| \widehat{O}_{\{\alpha_j\}} (|\{i_n\}\rangle \langle\{i_n\}| - |\{i'_n\}\rangle \langle\{i'_n\}|) \right| \Psi^* \right\rangle \right|^2 \tag{129}$$

with

$$\sum_{set} := \sum_{i\in\{\alpha_j\}} \sum_{l_i=1}^{d_i-1} \sum_{k_i<l_i} \sum_{\{i_n\}\neq\{i'_n\}} . \tag{130}$$

The indices l_i and k_i belong to the flip operator $\widehat{O}_{\{\alpha_j\}}$ defined in equation (123) . The entire amount of entanglement can be written as the sum of all m-concurrences, but so far this construction is only valid for pure states. Thus for a pure state $|\Psi\rangle$ or ρ_{pure}, respectively, its entanglement is equal to the sum of the squared mixedness of all subsystems:

$$E(|\Psi\rangle) := \sum_{m=2}^{n} C^2_m = \sum_{s=1}^{n} M^2(\rho_{pure,s}) \tag{131}$$

The extension to arbitrary states is done by the convex roof construction, that was introduced in the previous chapter 7.2. Hence when talking about the m-concurrence and the entanglement of a mixed state ρ, $(C^m_{(g)}(\rho))^2$, the greatest lower bound of all possible decompositions in pure states has to be calculated.

$$(C^m_{(g)}(\rho))^2 := \inf_{|\Psi_i\rangle,p_i} \sum_{|\Psi_i\rangle,p_i} p_i (C_{(m)}(|\Psi_i\rangle))^2 \tag{132}$$

Again the drawback of a convex roof measure is revealed when it comes to calculating the bounds. However inspired by Wootter´s and Hill´s concurrence

$$\tilde{\rho}^m_{\{\alpha_j\}} := O_{\{\alpha_j\}} (|\{i_n\}\rangle \langle\{i_n\}| - |\{i'_n\}\rangle \langle\{i'_n\}|) \rho^* O_{\{\alpha_j\}} (|\{i_n\}\rangle \langle\{i_n\}| - |\{i'_n\}\rangle \langle\{i'_n\}|), \tag{133}$$

can be constructed. Using the square roots of the eigenvalues of the matrix $\tilde{\rho}^m_{\{\alpha_j\}}\rho$, $\lambda^{\{\alpha_j\}}_m$, the resulting bounds look again similar to the previous case (110),

$$(B^m(\rho))^2 := \sum_{set} \sum_{\{\alpha_j\}} \max\left[0, 2\max\left[\left\{\lambda^{\{\alpha_j\}}_m\right\}\right] - \sum \left\{\lambda^{\{\alpha_j\}}_m\right\}\right]. \tag{134}$$

With this construction a useful entanglement measure is obtained. But it has to be noted that the current thoughts are not invariant under local unitary transformation (only in special cases) and therefore the m-concurrence is by implication not equal to the m-partite entanglement. However this problem can be corrected, as it stems from the fact that the m-concurrence involves also parts from $(m-i)$-concurrences (with $i < m$ and $(m-i) \geq 2$), by subducting these $(m-i)$-concurrences. This again restores the recommended invariance under local unitary transformation. For further informations about this m-concurrence measure it is referred to reference [65], whereas special examples on how this measure can be found in the upcoming chapters of this work or the eligible references.

[47] There are $\binom{n}{m}$ possible combinations.

CHAPTER 8

Entanglement Witness

The last separability criterion, that is discussed in this thesis, are the so called *entanglement witnesses*. This is maybe one of the more intuitive criteria, since it can be based on geometrical consideration. Regarding the convex set of separable states, surrounded by the set of entangled states, the region of separability or the borders of it, respectively, can be characterized by hyperplanes, that are tangential or at least near to the surface of this region (Hahn-Banach Theorem). This leads to a separation of the entire Hilbert space into two parts (Figure 7). Mathematically these hyperplanes are given by positive (P) or completely positive (CP) maps leading between the eligible Hilbert spaces or operators acting on it (compare chapter 1). Even though this work focuses on entanglement witnesses as operators acting on a bipartite system, a short outlook on p and cp maps as well as on the generalization to multipartite systems shall be given following the works of [5, 67, 6].

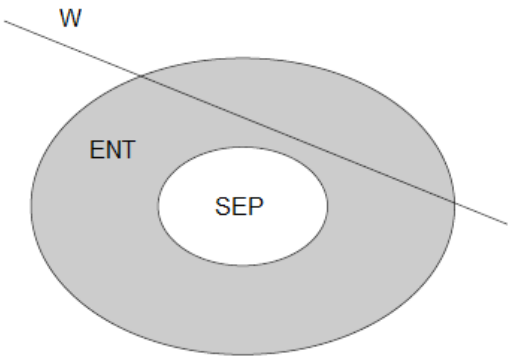


Figure 7: Entanglement witness W as a Hyperplane in Hilbert space

Definition (Entanglement Witness):
An operator W is called entanglement witness for an arbitrary pure or mixed state $\rho \in \mathcal{H}_A^{d_1} \otimes \mathcal{H}_B^{d_2}$, if

$$\langle W\rho_s \rangle = Tr(W\rho_s) \geq 0 \quad \forall \rho_s \in SEP \tag{135}$$
$$\langle W\rho_e \rangle = Tr(W\rho_e) < 0 \quad \forall \rho_e \notin SEP \tag{136}$$

A state is said to be detected by an entanglement witness, iff the latter inequality holds. For an operator W_t sufficing $Tr(W_t\rho_s) = 0$, the witness is called a tangential witness, as the corresponding hyperplane lies right on the surface of SEP, otherwise for $Tr(W\rho_s) > 0$ ($Tr(W\rho_s) < 0$) the hyperplanes is inside (outside) the set of entangled states (ENT). This obvious geometrically observation has its mathematical analogy in the Hahn-Banach Theorem, which also proves [32] that each entangled state is detected by at least one witness.

8.1 Construction of Witnesses

With this "completeness " relation the next step would be the construction of such a suitable witness for every state. In order to do that it is useful to distinguish between two kinds of witnesses, decomposable and non decomposable:
Definition (decomposable witness):
A bipartite entanglement witness $\mathcal{W}$, that is an element of the set of all bounded operators $\mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$, is called decomposable, if it can be written as

$$\mathcal{W} = P + Q^{T_B} \tag{137}$$

with P and Q being positive operators and Q^{T_B} denotes the partial transposition of Q in subsystem B.

This classification has its origin in the theory of P but not CP map, or more precise a decomposable map $\Lambda^{dec} \in \mathcal{B}(\mathbb{C}^2) \to \mathcal{B}(\mathcal{H}^2)$ or $\mathcal{B}(\mathcal{H}^2) \to \mathcal{B}(\mathcal{H}^3)$, that is of the form $\Lambda^{dec} = \Lambda^{(1)}_{CP} + \Lambda^{(1)}_{CP} \circ T$, where $\Lambda^{(i)}_{CP}$ is a CP map and T the transposition operator (see reference [5]), which are directly connected to operator witnesses itself (Choi-Jamiolkowski isomorphism in chapter 1)
This means that the same definition as before can be posed using PnCP maps:
For a state $\rho \in \mathcal{H}^d_A \otimes \mathcal{H}^d_B$ and the map $(\mathbb{1} \otimes \Lambda)[\rho]$, with $\Lambda : \mathcal{H}^d_A \to \mathcal{H}^d_B$ being a PnCP map the following inequalities hold:

$$Tr[(\mathbb{1} \otimes \Lambda)\ [P^+_d]\ \rho_s] \geq 0 \quad \forall \rho_s \in SEP \tag{138}$$

$$Tr[(\mathbb{1} \otimes \Lambda)\ [P^+_d]\ \rho_s] < 0 \quad \forall \rho_e \notin SEP \tag{139}$$

P^+_d denotes the projector on the pure maximally entangled state $\left|\Psi^+_d\right\rangle = \frac{1}{d}\sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle$ [48]. Therefore compared with (135) and (136), respectively, the connection between the operator witness and the CnCP map witness is given by $\mathcal{W} = (\mathbb{1} \otimes \Lambda)[P^+_d]$, whereas also the inverse relation $\Lambda = Tr_B[\mathcal{W}\rho^T] \otimes \mathbb{1}_d$ is sometimes useful.
This isomorphism is an important issue for the construction of witnesses, since a lot of separability or entanglement criteria are based on P or CP maps, e.g. as it was stated in chapter 4, in which the partial transposition criterion was introduced. This implies that for all these kinds of criteria a suitable witness can be constructed. A simple example of such a construction gives a state ρ_e, that is revealed to be entangled by the pt-criteria, i.e. due to the partial transposed density operator $\rho_e^{T_A}$ there exists at least one eigenvector $|\kappa\rangle$ with corresponding eigenvalue $\lambda_\kappa < 0$. The suitable witness is given by the outer product of this eigenvector, $W_{\rho_e} := |\kappa\rangle\langle\kappa|^{T_A}$. With the previous definition of an entanglement witness follows obviously

$$Tr(W_{\rho_e}\rho_e) = Tr(|\kappa\rangle\langle\kappa|^{T_A}\ \rho_e) = Tr(|\kappa\rangle\langle\kappa|\ \rho_e^{T_A}) = \lambda_\kappa < 0, \tag{140}$$

i.e. ρ_e is indeed an element of the set of entangled states. On the other hand a separable states ρ_s is, as expected, also recognized via $Tr(|\kappa\rangle\langle\kappa|\ \rho_s^{T_A}) > 0$.

Another interesting construction method uses the fact that the neighborhood of an already known pure entangled state $\rho_e = |\kappa\rangle\langle\kappa|$ comprises again entangled states. The arising question is, how much noise can be added to this state until it ends up in the set of separable states, or the other way round, how much noise is required, when a pure entangled state is subtracted until the region of entanglement is obtained:

$$\mathcal{W} := \alpha\mathbb{1} - |\kappa\rangle\langle\kappa| \tag{141}$$

In order to determine the minimal weight α, which provides that all separable states fulfill equation (134), it has to be assumed, that $Tr[\mathcal{W}\rho_s] = Tr[(\alpha\mathbb{1} - |\kappa\rangle\langle\kappa|)\rho_s] = \alpha - Tr[|\kappa\rangle\langle\kappa|)\rho_s]$ is equal zero for the largest value $Tr[|\kappa\rangle\langle\kappa|)\rho_s]$, which depends on certain separable states. Considering that the trace is a linear functional, which takes its maximum over a convex set, as in this case SEP, on its largest points, the eligible states ρ_s are all pure product states. That means that the proportion of noise is given by

$$\alpha = \max_{\rho_s} Tr[|\kappa\rangle\langle\kappa|\ \rho_s] = \max_{|\Phi\rangle=|A\rangle\otimes|B\rangle} Tr[|\kappa\rangle\langle\kappa|\ |\Phi\rangle\langle\Phi|] = \max_{|\Phi\rangle=|A\rangle\otimes|B\rangle} |\langle\kappa|\Phi\rangle|^2, \tag{142}$$

which is the square root of the largest Schmidt coefficient of $|\kappa\rangle$.

[48] The normalization factor can also be omitted, as it is done in reference [6].

A further enhancement of such deliberations are the so called *geometrical witnesses*, that require the definition of the Hilbert-Schmidt Norm of an operator, $\|X\|_{HS} := \sqrt{Tr(X^\dagger X)}$. This norm defines the distance between an entangled state ρ_e and the closest separable state ρ_s (compare references [68, 69]). The witness $\mathcal{W}$ is then constructed in such a way that it is optimal for all states along the connection between ρ_e and ρ_s (here called ρ_{line}), $Tr[\mathcal{W}\rho_{line}] = 0$:

$$\mathcal{W} := \frac{1}{\|\rho_e - \rho_s\|}(\rho_s - \rho_e + Tr[\rho_s(\rho_e - \rho_s)]\mathbb{1}) \tag{143}$$

Most of the existing methods of witness construction are closely related to other criteria due to the previously introduced isomorphism to PnCP maps, which seem to be the underlying theory behind these criteria.

8.2 Optimization

For an improvement of a given witness one has to define some kind of 'value' for it [70]. Therefore a witness $\mathcal{W}_1$ is called *finer* than a witness $\mathcal{W}_2$ if $\mathcal{W}_1$ detects more states than $\mathcal{W}_2$ in the sense that all states detected by $\mathcal{W}_2$ are also detected. A logical consequence for such witnesses is

$$\mathcal{W}_2 = \mathcal{W}_1 + P, \tag{144}$$

with P being some positive operator. Furthermore a witness $\mathcal{W}_o$ is called a optimal witness if $P = 0$ for all other eligible witnesses, or using the latter definition: There is no witness finer than $\mathcal{W}_o$ (if there would be a finer witness $W_f = W_o + P$, for some $P \neq 0$ W_f would not be a witness anymore).
For the optimization itself one has to distinguish between decomposable (d) and non decomposable (nd) witnesses. Regardless of this discrimination the set of product states on which a witness W vanishes is useful to define:

$$p_{\mathcal{W}} := \{|a,b\rangle \in \mathcal{H}| \langle a,b| \mathcal{W} |a,b\rangle = 0\}, \quad \text{with } |a,b\rangle \in \mathcal{H}_A^{d_1} \otimes \mathcal{H}_B^{d_2} \tag{145}$$

Based on these definitions an optimization or an iteration, respectively, can be introduced for d as well as for nd entanglement witnesses. The following theorems can be posed, based on the fact, that a finer entanglement witness can be obtained by subtracting projectors, that are characterized by a vanishing expectation value with elements of the the set p_W, or more precisely:
Theorem (Optimization of decomposable entanglement witnesses):
If, for a given d entanglement witness $\mathcal{W}$, a projector P, such that $PP_{\mathcal{W}} = 0$ [49] and furthermore a corresponding scalar factor λ_0, given by

$$\begin{aligned}\lambda_0 :&= \inf_{|a\rangle \in \mathcal{H}_a} \left[\langle a| P |a\rangle^{-\frac{1}{2}} \langle a| W |a\rangle \langle a| P |a\rangle^{-\frac{1}{2}} \right]_{\min} \\ &= \left(\sup_{|a\rangle \in \mathcal{H}_a} \left[\langle a| W |a\rangle^{-\frac{1}{2}} \langle a| P |a\rangle \langle a| W |a\rangle^{-\frac{1}{2}} \right]_{\max} \right)^{-1} > 0,\end{aligned} \tag{146}$$

[49] $P_{\mathcal{W}}$ denotes the projector on the set p_W and therefore $PP_{\mathcal{W}} = 0$ is equivalent to $\langle a,b| P |a,b\rangle = 0$.

can be found [50], then, iff $\lambda < \lambda_0$ and $\lambda > 0$, an entanglement witness

$$\mathcal{W}'(\lambda) := \frac{\mathcal{W} - \lambda P}{1 - \lambda} \tag{147}$$

can be constructed, which is finer then $\mathcal{W}$.
This theorem can be used iteratively:

- Determine $p_{\mathcal{W}}$
- Finding an operator $PP_{\mathcal{W}} = 0$ and a corresponding λ_0
- Defining a finer witness as $\mathcal{W}'(\lambda) := \frac{\mathcal{W} - \lambda P}{1-\lambda}$, with $\lambda \neq 0$ and $\lambda \leq \lambda_0$
- Set $\mathcal{W}' := W$ and start with point 1

With a simple modification of the projector P, an analogue method can be introduced for nd-witnesses:
Theorem (Optimization of non decomposable entanglement witnesses):
If there exists for a nd entanglement witness $\mathcal{W}$ a nd operator D, such that $DP_{\mathcal{W}} = 0$ and again a corresponding scalar factor λ_0,

$$\begin{aligned} \lambda_0 :&= \inf_{|a\rangle \in \mathcal{H}_a} \left[\langle a| D |a\rangle^{-\frac{1}{2}} \langle a| W |a\rangle \langle a| D |a\rangle^{-\frac{1}{2}} \right]_{\min} \\ &= \left(\sup_{|a\rangle \in \mathcal{H}_a} \left[\langle a| W |a\rangle^{-\frac{1}{2}} \langle a| D |a\rangle \langle a| W |a\rangle^{-\frac{1}{2}} \right]_{\max} \right)^{-1} > 0, \end{aligned} \tag{148}$$

then iff, $\lambda < \lambda_0$ and $\lambda > 0$, a nd entanglement witness

$$\mathcal{W}'(\lambda) := \frac{\mathcal{W} - \lambda D}{1 - \lambda} \tag{149}$$

can be constructed, which is finer then $\mathcal{W}$.
This theorem can also be used iteratively:

- Determine $p_{\mathcal{W}}$ and $p_{\mathcal{W}^T}$
- Finding an operator D given by $D = aP + (1-a)Q^T$ with $a \in [0,1]$, $PP_W = 0$ and $QP_{W^T} = 0$, and calculating λ_0
- Defining a finer witness as $\mathcal{W}'(\lambda) := \frac{\mathcal{W} - \lambda D}{1-\lambda}$, with $\lambda \neq 0$ and $\lambda \leq \lambda_0$
- Set $\mathcal{W}' := W$ and start with point 1

These iterations come to an end when no further Projector P can be subtracted from $\mathcal{W}$ or $\lambda_0 = 0$, respectively, and the optimal witness operator is found.

The drawback of these optimization method is that whenever a d or nd witness is used in order to find a optimal one, the resulting witness does not preserve this property itself. This means that the optimal witness of a previously decomposable one could then have the form

[50] $[\ldots]_{max/min}$ stands for the maximal/minimal eigenvalue and $X^{-\frac{1}{2}}$ is the the square root of the pseudo inverse operator of X^P. (X^P is called the pseudo inverse of a bounded operator X with a closed image if $X^P |\Psi\rangle = |\Phi\rangle \Leftrightarrow \| X |\Phi\rangle - |\Psi\rangle \| \to \min$ when $\| |\Phi\rangle \| \to \min$.)

of a non decomposable witness and vice versa. In order to solve this problem a so called *edge state* δ, located on the surface of the surface of PPTES (the set of PPT states), is defined:

$$\delta - \epsilon \left|a,b\right\rangle \left\langle a,b\right| \quad \notin \text{PPTES} \qquad \forall \left|a,b\right\rangle \in \mathcal{H}^{d_1} \otimes \mathcal{H}^{d_2}. \tag{150}$$

Furthermore every state $\rho \in$ PPTES can be presented as a convex combination of a separable and an edge state: $\rho = (1-p)\rho_{sep} + p\delta$. The use of this definition can be seen when looking at the characterization of states. Edge states are elements of the set, that is located in between SEP and PPTES and therefore vanish as long as $\rho \in \mathcal{H}^d$ with $d \leq 6$, because of the necessary and sufficient property of the pt-operation in this dimensions. I.e. for states with dimension six or lower the above presented witness $\mathcal{W}_{\rho_e}$ is the optimal one. For higher dimensions this gap, that contains entangled ppt states, has to be investigated. The states, lying in the gap, can only be detected by nd witnesses , contrarily to separable states. A possible construction of these nd-witnesses was found by Lewenstein et. al. [71]:
Any nd witness $\mathcal{W}$, detecting some edge state δ, which comprises in its range product states, denoted by $|a,b\rangle$ ($|a,b\rangle \in R(\rho)$), whereas $|a,b^*\rangle \in R(\rho^{T_B})$, can be expressed as

$$W = P + Q^{T_B} - \epsilon \mathbb{1}, \quad \text{with} \quad 0 \leq \epsilon \leq \inf_{|a,b\rangle} \left\langle ab|(P + Q^{T_B}|ab\right\rangle, \tag{151}$$

with $P, Q \geq 0$ and $R(P) \subseteq K(\delta)$, $R(Q) \subseteq K(\delta^{T_B})$. With this nd witness of an edge state and the above stated optimization theorem all ingredients are given in order to build an optimal entanglement witness, which exactly distinguishes between separable and entangled states.
Further useful results or other approaches to this optimization problem can be found in reference [70], e.g. an optimal witness W_o the already mentioned product states $|a,b\rangle$, have to span the entire Hilbert space as well as $\langle a_i, b_i|W_o|a_i, b_i\rangle = 0$ has to be fulfilled.

8.3 Bell inequalities - a special kind of witness

Another interesting aspect of witnesses is the connection to Bell inequalities, which shows nicely the fluent border between the different methods in characterizing quantum states. This result was found by Barbara M. Terhal [72]. Considering again the theory of Bell inequalities (chapter 3) for a bipartite system. A given state ρ, that is shared by two parties, Alice and Bob, is called nonlocal when its expectation value with the Bell operator violates a certain bound. Along with this nonlocality comes a special correlation between Alice and Bob, that could not be described by the assumption of hidden variables. Usually the highest violation of this bound and therefore the most nonlocal features depends on how the Bell inequality was constructed and for which states it is optimized. Hence when assuming the situation that each party is sharing a mixed or separable state, which could in the first instance not violate a Bell inequality, its nonlocality can often be increased by allowing Alice and Bob to use LOCC operations (chapter 1) on his or her substate. This is nothing else but the previously introduced distillation (chapter 6), which allows to transform every mixed or separable state into a certain entangled singlet, that also has nonlocal properties. However for showing the connection between Bell inequalities and entanglement witnesses a set of measurement operators for Alice, M_i^A, $i = 1, ..., n_A$ and Bob, M_j^B, $j = 1, ..., n_B$, is assumed. Each operator used by Alice has the substructure

$$M_i^A := (E_{i,1}^A, E_{i,2}^A, ..., E_{i,k(i)}^A), \quad \text{with} \sum_{m=1}^{k(i)} E_{i,m}^A = 1, \; E_{i,m}^A \geq 0 \tag{152}$$

with $E^A_{i,k}$ being the positive operator corresponding to the k-th measurement outcome of the i-th operator M^A_i on Alice´s side. The same definitions are valid for Bob´s subsystem. A so called probability vector $\vec{P}$ can now be constructed comprising the possible measurement results of both subsystems, $P_{A:i|k} = Tr\left[E^A_{i,k} \otimes \mathbb{1}\rho\right]$ and $P_{B:j|l} = Tr\left[\mathbb{1} \otimes E^B_{j,l}\rho\right]$, as well as the correlated measurement results, $P_{A:i|k,B:j|l} = Tr\left[E^A_{i,k} \otimes E^B_{j,l}\rho\right]$:

$$\vec{P} := \begin{pmatrix} P_{A:i|k,B:j|l} \\ P_{A:i|k} \\ P_{B:j|l} \end{pmatrix} \tag{153}$$

The size of this vector varies according to the number of measurement operators and outcomes on each subsystem and can be associated with a certain set of so called *Boolean vectors* [51]. This is done by assuming a hidden variable λ that can either be 0 or 1 for a certain measurement outcome, i.e. it is measured with probability one or zero. Hence every eligible outcome scenario can be referred to a special Boolean vector $\vec{B}_\lambda$ and every measurement set-up to the corresponding set of Boolean vectors. That means also that $\vec{P}$ can be associated with

$$\vec{B}_\lambda := \begin{pmatrix} \vec{B}^A_\lambda \otimes \vec{B}^B_\lambda \\ \vec{B}^A_\lambda \\ \vec{B}^B_\lambda \end{pmatrix}, \tag{154}$$

with $\vec{B}_\lambda$ describing only one single outcome scenario and therefore the complete system is described by the set $\vec{B}_{\lambda_1}, ..., \vec{B}_{\lambda_N}$, whereas N denotes the number of all possible Boolean vectors of $\vec{B}^A_\lambda$ and $\vec{B}^B_\lambda$. Relating to this, every LHV-Theory can be connected to a convex combination of the eligible set of Boolean vectors $\vec{B}_{\lambda_i}$ vector $\vec{V}$,

$$\vec{V} = \sum_i q_i \vec{B}_{\lambda_i}, \quad \text{with} \quad q_i \geq 0. \tag{155}$$

Represented in a more general way by vectors of positive numbers $\vec{P}^A_i$ and $\vec{P}^B_i$, respectively, $\vec{V}$ can be represented as

$$\vec{V} := \sum_i p_i \begin{pmatrix} \vec{P}^A_i \otimes \vec{P}^B_i \\ \vec{P}^A_i \\ \vec{P}^B_i \end{pmatrix}. \tag{156}$$

That means that this set of all LHV-Theories $\mathcal{L}_{LHV}(M)$ is a convex cone spanning a vector space that is one to one correlated to a simplex in the Hilbert space, that consists of all states obeying the LHV theory. It has to be noted that this convex cone and hence the corresponding simplex depends on the actual measurement operators (M^A_i and M^B_i) prepared by Alice and

[51] This denotes a vector, whose elements are either 0 or 1.

Bob. If a state ρ, that is measured by Alice and Bob is describable by such a vector $\vec{V}$, it fulfills a LHV-Theory. I.e. by checking whether the vector $\vec{V}$, that corresponds to the measured state ρ, is element of $\mathcal{L}_{LHV}(M)$, the nonlocality of a state can be detected. Via the so called *Minkowski-Farkas Lemma* [73] for convex sets in $\mathbb{R}^n$ a more precise constraint can be given concerning the states inside this simplex by denoting whether a vector $\vec{P}$ is element of $\mathcal{L}_{LHV(\mathcal{M})}$ or not. The latter is true iff there exists a vector $\vec{F}$ [52] such that

$$\vec{F} \cdot \vec{P} < 0 \quad \text{and} \quad \vec{F} \cdot \vec{B}_{\lambda_i} \geq 0 \; \forall \lambda_i. \tag{157}$$

This formulation of finding a suitable $\vec{F}$ for a state ρ is nothing else but constructing a Bell inequality, which is violated by the very same state ρ. For a bipartite entangled state the vector $\vec{F}$ can be chosen as $\vec{F} = (F_{A:i|k,B:j|l}, F_{A:i|k}, F_{B:j|l})^T$ and an operator can be constructed by

$$H := \sum_{i,j,k,l} F_{A:i|k,B:j|l} E^A_{i,k} \otimes E^B_{j,l} + \sum_{i,k} F_{A:i|k} E^A_{i,k} \otimes \mathbb{1} \sum_{j,l} F_{B:j|l} \mathbb{1} \otimes E^B_{j,l} \tag{158}$$

that heads back to the familiar Bell operator form $\vec{F} \cdot \vec{P} = TrH\rho \leq 0$. For spin measurements with the Pauli operators H reduces to

$$H = \frac{1}{4}(21 - \vec{a}\vec{\sigma} \otimes (\vec{b} + \vec{b'})\vec{\sigma} - \vec{a'}\vec{\sigma} \otimes (\vec{b'} - \vec{b})\vec{\sigma}) \tag{159}$$

which is equivalent to the operator found for the CHSH inequality (chapter 3).

[52] $\vec{F}$ stands for the Farkas vector.

Part III
Geometry of Qudits

The next chapters are dealing with the task of visualizing and drawing geometrical pictures of quantum states regarding their different properties. This is possible, since in special cases every quantum state, which is an element of the abstract Hilbert space, can be uniquely identified with a point in the Euclidean vector space. This opens a lot of possibilities, such as introducing a metric based on distance or geometrical witnesses, that can be used to detect entanglement or an easy way of comparing the strength of different separability criteria. In order to get such images it is necessary to restrict the amount of different quantum states with constraints by limiting the number of particles or reducing their degrees of freedom. This is done by writing states, which are eligible candidates for visualizations, with real valued parameters, that can be used as variables for a geometrical illustration. The next chapter shows how this is done in the easiest, the bipartite qubit case.

CHAPTER 9

Bipartite Qubits

In the two qubit case, $\mathcal{H}_A^2 \otimes \mathcal{H}_B^2$, the states can be written by using the canonical basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ as

$$|\Psi\rangle = p_{1,0}\ p_{2,0}\,|00\rangle + p_{1,0}\ p_{2,1}\,|01\rangle + p_{1,1}\ p_{2,0}\,|10\rangle + p_{1,1}\ p_{2,1}\,|11\rangle\,, \tag{160}$$

with the four variables $p_{i,j}$ representing the weights corresponding of the j-th basis vector, $j \in \{0,1\}$ of the i-th qubit, $i \in \{0,1\}$. The density operator $|\Psi\rangle\langle\Psi|$ consists of 16 matrix elements, the products of the $p_{i,j}$´s. Using the the Bell operator base $\{\mathbb{1}, \sigma_1, \sigma_2, \sigma_3\}$ and the Bloch representation of qubits, respectively, one receives

$$|\Psi\rangle\langle\Psi| = \rho = \frac{1}{2}(\mathbb{1} + a_i\ \sigma_i) \otimes \frac{1}{2}(1 + b_j\ \sigma_j) = \frac{1}{4}(\mathbb{1}\otimes\mathbb{1} + a_i\ \mathbb{1}\otimes\sigma_i + b_j\ \sigma_j\otimes\mathbb{1} + c_{ij}\ \sigma_i\otimes\sigma_j), \tag{161}$$

whereas the variables are represented by entries of the the real vectors $\vec{a} = (a_1, a_2, a_3)^T$, $\vec{b} = (b_1, b_2, b_3)^T$ and the matrix $c_{ij} = a_i b_j$ [53]. Following the work of [48] a picture can be drawn by reducing these variables to at least three. This is done by regarding only locally maximally mixed states (i.e. $Tr_i\rho = 1$, $i \in \{A, B\}$), such that the coefficients a_i and b_j vanish. The only thing we are left with are the entries c_{ij} of a 3×3 matrix, that we can simplify by singular value decomposition [54]. The remaining states are given by

$$\rho = \frac{1}{2}(\mathbb{1}\otimes\mathbb{1} + \sum_{i=1}^{3} c_i\ \sigma_i \otimes \sigma_i). \tag{162}$$

The three coefficients c_i can now be used as variables in order to to draw a three dimensional picture. The states have to fulfill the positivity condition $\rho > 0$, which means $|c_i| \geq 0$.

[53] The three variables a_i and b_i, respectively, of each qubit are reduced to two by $Tr(\rho) = 1$.

[54] This is possible, since of the sigma base can be uniquely referred to a three dimensional euclidean vector $(\sigma_1\ \sigma_2\ \sigma_3)^T$. Or more fundamental the Isomorphism between the SU(2) and O(3).

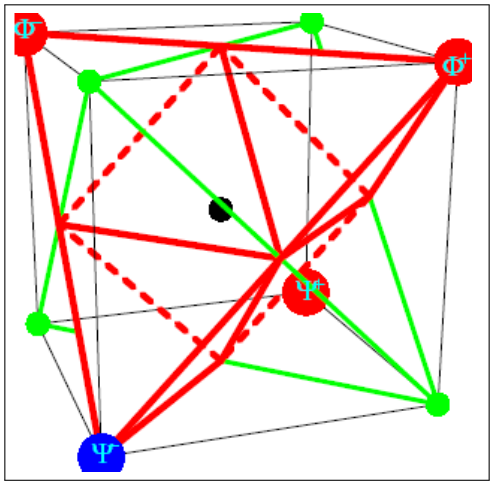


Figure 8: Geometry of two qubits

Moreover the c_i indicate uniquely, by applying the Peres-Horodecki criterion, where the separated and entangled regions of this states can be found. With this constraints the following picture of a tetrahedron is received (Figure 8).
At the edges of this tetrahedron the pure maximally entangled Bell states $|\Phi^{\pm}\rangle$ and $|\Psi^{\pm}\rangle$ can be found. Within the double pyramid all separable states are located.

CHAPTER 10

N-partite Qubits

This chapter is generalizing the previous results of two qubits by regarding a quantum system with an arbitrary but fixed number of qubits n (also known as the n-partite qubit case). An arbitrary state vector $|\Psi\rangle \in \mathcal{H}^{2n}$ describing such a system contains n entries, either 0 or 1. Following the well-established way of using the sigma operator basis, it can be written as:

$$\begin{aligned}\rho = & \frac{1}{2}(1 + c_i\sigma_i) \otimes \frac{1}{2}(1 + c_j\sigma_j) \otimes ... \otimes \frac{1}{2}(1 + c_n\sigma_n) \\ = & \frac{1}{2^n}\Big((1 \otimes 1 \otimes ... \otimes 1) + a_{jk...n}(1 \otimes \sigma_j \otimes \sigma_k \otimes ... \otimes \sigma_n) + b_{ik...n}(\sigma_i \otimes 1 \otimes \sigma_k \otimes ... \otimes \sigma_n) + ... \\ & + c_{ij...n}(\sigma_i \otimes \sigma_j \otimes ... \otimes \sigma_n)\Big) \end{aligned} \tag{163}$$

Again all parameters $a_{jk...n}, b_{ik...n}, ...$, except for $c_{ij,...,n}$, are vanishing, when these states are restricted to locally maximal states. The result is, as in the previous chapter, $Tr_{\neg i}\rho = 1$ [55] as well as $Tr_{\neg i,j}\rho = 1, Tr_{\neg i,j,k}\rho = 1, ..., Tr_{\neg i,j,..,n-1}\rho = 1$. Also the remaining parameters $c_{i,j,...,n}$ of this matrix can be handled as in the two qubit case, such that via singular value decomposition the three variables c_i remain.

Since the same strategy as in the bipartite case was used the locally maximally mixed n-qubit states have the same pattern as in the two qubit case:

[55] The trace is taken over all possible subsystems except the j-th subsystem.

$$\rho = \frac{1}{2^n}(1 + \sum c_i \sigma_i^{\otimes n}) \tag{164}$$

Now it is possible to give a geometrical picture with the three variables c_i by applying the methods introduced in previous sections:

i) **Positivity of the states**

By investigating the positivity of ρ it turns out that one has to distinguish between an odd and an even number of particles:

a) If n is odd, the positivity is given by $|c_i|^2 \leq 1$

b) If n is even, the positivity is given by

$$(1 - \vec{c}.\vec{n_i}) \geq 0, \quad \text{where the vectors } \vec{n}_i \text{ are } \begin{pmatrix} -1 \\ +1 \\ +1 \end{pmatrix} \begin{pmatrix} +1 \\ -1 \\ +1 \end{pmatrix} \begin{pmatrix} +1 \\ +1 \\ -1 \end{pmatrix} \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix} \tag{165}$$

This means from a geometric point of view, that an odd amount of qubits lies within the Bloch Sphere, whereas for an even number of particles the same geometry as in the two qubit case is received, namely the tetrahedron, given by the four planes of the vectors $\vec{n}_i$.

ii) **pt-criterion**
In order to find the regions of separability the states are scrutinized with the pt-criterion. It interchanges the basis vectors of the ρ in each subsystem. Reordering the subsystems, that consist of the identity matrix and the Pauli matrices, according to the pt criterion is equal to switching the off-diagonal elements of this four matrices. The result of this is therefore a change of sign of the σ_y matrix. Hence also the separability depends on whether the number of particles is even or odd.

a) For n being an odd number the pt-criterion leads to sign change of the whole state: $\rho^{pt} = -\rho$.
The result however coincides with the positivity criterion $|c_i|^2 \leq 1$, which is obvious since the sign does not affect the absolute value of $\vec{c}$. So according to the pt-criterion all states inside the positivity sphere are entangled.

b) For n being an even number the sign change has no effects on the state, i.e. $\rho^{pt} = \rho$
Also for even number of particles the region of entangled states is given by the bounds of the positivity, $(1 - \vec{c}.\vec{n_i}) \geq 0$.
Contrary to the positivity this equation allows an additional tetrahedron, mirrored to the other one, such that the intersection forms an octahedron in which all ppt states are located

However it must be considered that the pt-criterion for this high dimensional problem is only a necessary and no sufficient criterion for entanglement. So the ppt states inside the octahedron might be entangled as well.
In order to find whether the state is entangled and between which subsystems entanglement

can be found, a multipartite entanglement measure (chapter 7.3) is used. Since the geometry for an odd amount of particles is rather trivial, it will be neglected in the following.

iii) **multipartite entanglement measure**

The measure allows to determine, which and how many parties are entangled with each other. So the total amount of entanglement is composed by

$$E(\rho) = E_2(\rho) + E_3(\rho) + ... + E_n(\rho) \tag{166}$$

where the $E_i(\rho)$ are called the i-partite Entanglement, expressing that i subsystems are entangled. This obviously leads to the substructure of

$$\begin{aligned} E_2(\rho) &= E_{1,2}(\rho) + E_{1,3}(\rho) + ... + E_{n-1,n}(\rho), \\ E_3(\rho) &= E_{1,2,3}(\rho) + E_{1,2,4}(\rho) + ... + E_{n-2,n-1,n}(\rho), \\ ... &= ... \\ E_n(\rho) &= E_{1,2,...,n}(\rho) \end{aligned} \tag{167}$$

For the states under investigation the only non vanishing entanglement is the n-partite entanglement E_n, which is a expected result, since by construction all local parameters were set to zero. The values of the bounds (compare equation (134)), are exactly the same as in the pt-criterion:

$$E_n = E_{1,2,...,n} = Xmax\Big[0, \frac{1}{2} max\left[-1 + \vec{c}\cdot\vec{n}^1, -1 + \vec{c}\cdot\vec{n}^2, -1 + \vec{c}\cdot\vec{n}^3, -1 + \vec{c}\cdot\vec{n}^4\right]\Big]^2 \tag{168}$$

The letter X distinguishes between the two qubit (here $X = 2$) and and the the $n > 2$ qubit case (here $X = 1$). The explanation of this difference lies in the generalization of maximally entangled states to higher dimension. For the purest states ($|c_i|^2 = 1$), that are located at the edges of the tetrahedron, the entanglement is maximal. For the bipartite case these states are the Bell states. When reconsidering how this measure was constructed, the maximal entanglement value of an n-partite system is n. This is given when all local obtainable information S is zero as well as the lack of classical knowledge R of the state (compare Bohr complementary relation (116)), which is the case for the two qubit Bell states. The n qubit states are also constructed in such a way that no information is available by regarding one subsystem (setting the traces over all subsystems except one to zero). This means $S = 0$ is fulfilled, but when going further and restricting also the information that could be received by two or more subsystems together (setting the traces over all subsystems except two, three, ...,n-1 to zero), the lack of classical knowledge R does not disappear. Therefore these states can not be called maximally entangled for $n > 2$, as they obey

$$n = E_n + R = 1 + R, \tag{169}$$

where R is a nonzero value, given for the edge states of the simplex by $R = n - E_n$.
Coming back to the result (169) one sees that the lower bounds of this measure give exactly the same octahedron, that is already known as the inner shape of the two tetrahedrons in the bipartite qubit case. According to this measure all state within this octahedron are separable with respect n-2 cuts, i.e. the amount of entanglement does not vanish when all n particles are investigated. How the measure for this states is constructed in detail can be seen in the Appendix.
A more exciting question to answer is whether the n partite entanglement can be distilled to a pure state, for $n = 2$, or to at least a more purer or the purest state, for $n > 2$. Therefore

a distillation protocol might be useful.

iv) **Distillation**

The distillation protocol is a generalization of the 2 way protocol described in chapter 6.1. Obviously it is altered to an n way protocol such that every party will receive a copy of the original state on which the common operations are applied. As previously described the protocol works in three steps

I Copy the state and give each subsystem one copy:
Here the state is copied once to illustrate one cycle of the protocol.

$$\begin{aligned}\rho \longrightarrow \rho^{\otimes 2} &= \frac{1}{2^n}(1^{\otimes n} + \sum c_i \sigma_i^{\otimes n})^{\otimes 2} \\ &= \frac{1}{2^{2n}}\Big((1\otimes 1)^{\otimes n} + c_i(1\otimes\sigma_i)^{\otimes n} + c_j(\sigma_j\otimes 1)^{\otimes n} + c_{ij}(\sigma_i\otimes\sigma j)^{\otimes n}\Big)\end{aligned} \tag{170}$$

II Every subsystem applies an LOCC operation:
In order to distill a totally entangled singlet out of this state the U_{XOR} operation is used (see chapter 6.1). Here the $|\Phi^+\rangle$ state for two particles and the generalization of this state for higher dimensions are the aspired totally entangled singlets. Therefore the operator, that is applied by each party on its two subsystems (the original and the copy), can be explicitly written as

$$U_{XOR} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{171}$$

The copied system is then projected in the same direction in such a way that each party applies the projector $P = \frac{1}{2}(1+\sigma_z)$ on each of their copy-subsystem. Summarizing all operations the new state $\tilde{\rho}$ is obtained by

$$\tilde{\rho} = (1\otimes P)U_{XOR}\rho^{\otimes 2}(1\otimes P)^\dagger \tag{172}$$

III Investigation of the distilled state
After these operators were applied the new, distilled state $\tilde{\rho}$ has changed its vector $\vec{c}$:

$$\vec{c} = \begin{pmatrix} c_x \\ c_y \\ c_z \end{pmatrix} \longrightarrow \tilde{\vec{c}} = \begin{pmatrix} \frac{c_x^2+c_y^2}{1+c_x^2} \\ \frac{2c_xc_y}{1+c_x^2} \\ \frac{c_z}{1+c_x^2} \end{pmatrix} \tag{173}$$

This vector and its components, respectively, are responsible for the position in the Euclidean space. Therefore the distillation can be seen as a geometrical shift of the state (see Figure 9).

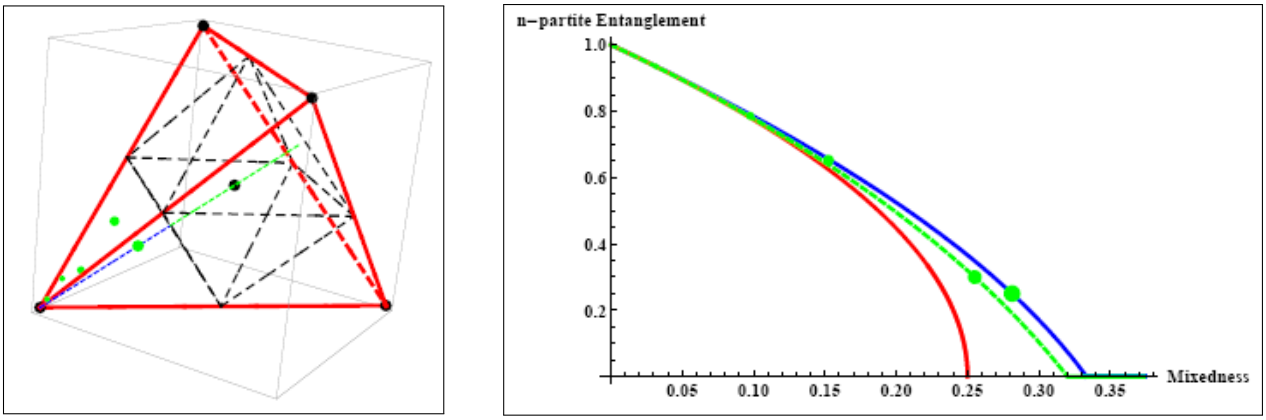
By running through this distillation circle several times the state is shifted more and more to one of the totally entangled edge states (in this case the $|\Phi^+\rangle$ state and its generalizations,

respectively). So obviously the amount of entanglement of the states inside the tetrahedron can be increased by this protocol up to a certain level. In order to determine this level exactly the generalized edge state singlets have to be inspected more precisely. Either the edge states are maximally entangled states, just like the Bell states for n=2, or, although they posses the highest level of entanglement in this simplex, they do not posses the maximal entanglement compared to all states in the $\mathcal{H}^{2n}$ Hilbert space. If the latter would be true the set of states in the tetrahedron would be bound entangled, otherwise distillable states.

For easier calculations of this problem, the four particle case ($n = 4$) is used as an example. The vertex or edge states of this simplex are characterized by $|\vec{c}|^2 = 3$. It can be shown that one of the four vertex states [56] is given by

$$\begin{aligned}\rho_{vertex1} =& \frac{1}{16}(1^{\otimes 4} + \sum c_i \sigma_i^{\otimes 4}) \\ =& \frac{1}{16}\Big\{(|0000\rangle + |1111\rangle)(\langle 0000| + \langle 1111|) + (|0011\rangle + |1100\rangle)(\langle 0011| + \langle 1100|) \\ &+ (|0101\rangle + |1010\rangle)(\langle 0101| + \langle 1010|) + (|1001\rangle + |0110\rangle)(\langle 1001| + \langle 0110|)\Big\} \quad (174)\end{aligned}$$

As one can see the state can be composed by four states, whereas the first is the GHZ state $\frac{1}{\sqrt{2}}|0000\rangle + |1111\rangle$ and the three others can be received by applying different state flips to this GHZ state [57]. This structure happens to be the case for all four vertex states.



Distillation

Distillation

Figure 9: Distillation of GHZ states

All partial states are totally entangled pure singlets, as they are unitary equivalent to the GHZ state, but the vertex state itself comprises a mixture of these state and is not pure anymore. The question whether the edge states are maximally entangled and what kind of entanglement they posses can therefore be answered: As mixtures of GHZ and unitary equivalent states they are no longer pure states. That means, as it is also detected by the measure, they carry n partite entanglement and as mixtures they can not be maximally entangled states. Nevertheless the vertex states posses the highest amount of entanglement compared to all states inside the simplex. And as the protocol can only distill entanglement up to the vertex states, which are not maximally entangled, all states inside the simplex are

[56] $c_1 = c_2 = c_3 = -1$
[57] $1 \otimes 1 \otimes \sigma_x \otimes \sigma_x, 1 \otimes \sigma_x \otimes \sigma_x \otimes 1, ...$

bound entangled.
For more detailed investigations, e.g. the exact proof of the separability of the states or why the bounds of the measure are exact, it is referred to the original paper in appendix B.

CHAPTER 11

A Simplex of W_k states

After a simplex comprising states, that consisted of states of the GHZ class and therefore poseses only n partite entanglement, it would be interesting to see whether it is also possible to visualize the other generalization of the maximally entangled Bell states, namely the W_k states. As the W_k state simplex would not only consist of W states and Dicke states, it is hard to say what kind of entanglement will be found and between which subsystems it will be located, which makes it worth considering. Obviously the answers to these questions depend, just like in the previous chapter, on how the simplex is constructed and which symmetries the set of states posses, i.e. which constraints are chosen to restrict the parameters in order to gain a geometrical structure.

The construction of an n partite qubit simplex consisting of W_k states is not as straight forward as in the previous chapter, in which the similar pattern to the bipartite qubit case could be used. Due to receiving a more different type of entanglement, compared to the GHZ simplex, the vertex states of the W_k simplex are modeled after the definition of the W_k states (equation (30)). This will lead to the fact, that for every amount of particles n, a different simplex is received. Therefore all dimensions have to be treated and analyzed differently, however, because of the same construction in general, commonalities will be elaborated. In the following two possible constructions of W_k-simplices are introduced, as after that, examples like the special cases of three and four particles systems are investigated and compared. However both constructions are founded on the same stand, that is introduced in the following:

N particle qubit states are elements of a $\mathcal{H}^{2n}$ Hilbert space and can be represented by the convex sum of elements of this set of states:

$$\mathcal{Z} := \{|ij...n\rangle\} \qquad \text{with} \quad i,j,...,n \in \{0,1\} \tag{175}$$

Because of the different permutation of 1 and 0, all elements z_i of $\mathcal{Z}$ are mutually orthogonal. By considering in how many ways k 1´s ($0 \leq k \leq n$) can be permuted on n positions, the number of elements z_i yields

$$\binom{n}{0} + \binom{n}{1} + ... + \binom{n}{n},\ 2^n \quad \text{possibilities}, \tag{176}$$

which makes $\mathcal{Z}$ to be a basis.
The construction of the simplex is completed, when n orthogonal vertex states, V_i, are found that are the basis states of the desired W_k simplex. However it has to be noted that the construction of these vertex states is not unique as these states consist of different superpositions comprising n of the possible 2^n states of the set $\mathcal{Z}$. There are two possible constructions leading to the known two qubit case when they are restricted to two particles.

11.1 The First Construction

This construction follows an intuitive way. W.l.o.g. the first vertex state, $|V_0\rangle$, is chosen as the W-state itself (31). Furthermore another vertex state, $|V_1\rangle$, can be built by taking n

additional states out of the set $\mathcal{Z}$ other than the ones that have been taken for the W state, i.e. states of the set $\mathcal{Z}$ / $\left\{ \left| \underbrace{10...0}_{n} \right\rangle, |010...0\rangle, ..., |000...1\rangle \right\}$. This leads to many possible combination and many vertex states, respectively, which are all unitary equivalent. In order to avoid confusion, the additional vertex states, $|V_i\rangle$ with $i > 0$, are received by a certain construction:
Considering an n particle system all other possible vertex states are received by starting with the $|V_0\rangle$, the W-state, on which the following operators are applied:

$$\begin{aligned} |V_1\rangle &:= \sigma_x \otimes \mathbb{1}^{\otimes n-1} |V_0\rangle \\ |V_2\rangle &:= \sigma_x^{\otimes n} |V_1\rangle \\ |V_3\rangle &:= \sigma_x \otimes \sigma_x \otimes \mathbb{1}^{\otimes n-2} |V_2\rangle \\ |V_4\rangle &:= \sigma_x^{\otimes n} |V_3\rangle \\ &\vdots \\ |V_{2i-1}\rangle &:= \sigma^{i+1} \otimes \mathbb{1}^{\otimes n-(i+1)} |V_{2i-2}\rangle \\ |V_{2i}\rangle &:= \sigma_x^{\otimes n} |V_{2i-1}\rangle \end{aligned} \tag{177}$$

In this construction $i < \frac{2^n}{n}$, with $i \in \mathbb{N}$. Therewith vertex states can be created until less than $2^n - n$ states $z_i \in \mathcal{Z}$ remain unused, as the remaining ones do not suffice to build another vertex state $|V_i\rangle$, i.e. a certain number of elements of $\mathcal{Z}$ (less then n), are not used. In this first construction it turns out that the dimension of the simplices are not equal to the dimension of the Hilbert spaces of the vertex states itself. This dimensional difference of constructed simplex and the Hilbert space differs due to the number of particles and hence due to the number of constructible vertex states. The two obvious possibilities occur:

- The number of particles n is a multiple of 2^n. Here $\frac{2^n}{n}$ vertex states can be constructed
- The number of particles n is a not multiple of 2^n. That means that $\lfloor \frac{2^n}{n} \rfloor$ [58] vertex states can be obtained and some of the $\{|ij...m\rangle\}$ states remain unused. Therefore already at this point it can be seen, that the resulting simplex will only be a subspace of the entire space, which is given by the basis $\mathcal{Z}$.

Considering the bipartite case, this construction would only give the two Bell states $|V_0\rangle := |\Psi^+\rangle$ and $|V_1\rangle := |\Phi^+\rangle$, respectively. In order to gain all Bell states, two new state with a different sign on the second term are required. Hence for an arbitrary amount of particles this sign change has to be generalized by adding proper [59] phases to the single basis states $\{|ij...m\rangle\}$, which build the vertex states. Proper means that the phases have to be chosen in such a way that that each vertex state is orthogonal to all other, $\langle V_i|V_j\rangle = 0$. Theses phases are obtained by dividing the complex unity circle into n equivalent parts. W.l.o.g the first phase is chosen to be 1, so the phases in general are

$$\alpha_k := e^{k\varphi_n} \qquad \text{with} \quad k \in \{0, 1, ..., n-1\} \quad \text{and} \quad \varphi_n := \frac{2\pi}{n}. \tag{178}$$

It is easy to see that for $n = 2$ the two eligible phases lead exactly to the $\pm$ sign changes on the second terms when the phases are multiplied with the states $|V_0\rangle$ and $|V_1\rangle$ is comprised, i.e. $\alpha_0 = e^{0\varphi_2} = 1$ attached to $|00\rangle$ and $\alpha_1 = e^{1\varphi_2} = -1$ to $|01\rangle$ and therefore the two missing

[58] The $\lfloor x \rfloor$ symbol denotes the next integer of x rounded down (compare Gaussian bracket $[x] = \max(\{k \in \mathbb{Z} | k \leq x)\}$).
[59] The phases are chosen in such a way that the states are all pairwise orthogonal.

Bell states, $|V_{0,1}\rangle := |\Psi^-\rangle$ and $|V_{1,1}\rangle := |\Phi^-\rangle$ are obtained.
However, the general n qubit situation is different. For creating new vertex states on a multi particle system similar to the bipartite case the existing vertex states $|V_j\rangle$, $1 \leq j \leq \left\lfloor \frac{2^n}{n} \right\rfloor$, can be doubled by adding the states $|V_{j,1}\rangle$:

$$|V_{j,1}\rangle = \sum_{\tilde{j}=0}^{n} \sigma_x^{\otimes \tilde{j}} \otimes \mathbb{1}^{\otimes n-\tilde{j}} \alpha_{0_1} \big| \underbrace{10...0}_{n} \big\rangle + \alpha_{1_1} |010...0\rangle + ... + \alpha_{(n-1)_1} |000...1\rangle \,, \tag{179}$$

with $j = \tilde{j}$ for $j \leq \left\lfloor \frac{2^n}{n} \right\rfloor$. The difference between the bipartite and the multiqubit case lies in the alignment of the phases α_i. Whereas in the bipartite case only one possible configuration, regardless overall phases, exists more permutations with respect to the mutual orthogonality are disposal in the general case. In order to mark the different phases α_{i_k} according to their arrangement of the current vertex state the index i specifies the affiliation to the pure states of the set $\mathcal{Z}$ as well as the lower index k refers to the k-th vertex state. In the notation $|V_{j,1}\rangle$ of the previous equation the index '1' denotes the first state, that contains the first, canonical phase arrangement. The number of vertex states and therefore the size of the simplex depends on how many of this phase combinations are possible (again neglecting rotations by overall phases). In order to find those and hence the existence of a further vertex states $|V_{j,2}\rangle$ the mutual orthogonality can be used. Since the orthogonality of the states $|V_{k,1}\rangle$ and $|V_k\rangle$, for $k \neq j$ can be seen immediately by the orthogonality of the elements of $\mathcal{Z}$, the crucial constraint is given by

$$0 = \langle V_{j,1}|V_{j,2}\rangle = \sum_{\Pi(j_2)=0}^{n-1} \sum_{i=0}^{n-1} \alpha_{i_1}^* \alpha_{j_2} = \sum_{\Pi(j_2)=0}^{n-1} \sum_{i=1}^{n-1} exp\left[(j_2 - i_1)\varphi_n\right] \quad \text{with} \quad i_1 \neq j_2. \tag{180}$$

$\sum_{\Pi(j_2)=0}^{n-1}$ denotes that the sum runs through all possible permutations of j_2´s from 0 to $n-1$. The j_2´s depend on the previously chosen phase arrangement of $|V_{j,1}\rangle$, which can be represented here as the sum from 0 to $n-1$. If a new phase arrangement, „j_2", can be found, a new vertex state,

$$|V_{j,2}\rangle = \sum_{\tilde{j}=0}^{n} \sigma_x^{\otimes \tilde{j}} \otimes \mathbb{1}^{\otimes n-\tilde{j}} \alpha_{0_2} \big| \underbrace{10...0}_{n} \big\rangle + \alpha_{1_2} |010...0\rangle + ... + \alpha_{(n-1)_2} |000...1\rangle \tag{181}$$

with $j = \tilde{j}$ for $j \leq \left\lfloor \frac{2^n}{n} \right\rfloor$, is gained. It has to be noted that the phase α_{0_2} is not equal to the value of α_0, as its index 'i_2' is only related to the value 'i' (equation (180)) for the first vertex state $|V_{j,1}\rangle$. The orthogonality constraint, that is posed in equation (179) in order to receive a new vertex state, is only true for the special case of receiving the $|V_{j,2}\rangle$ state. When this construction is iterated to get further vertex states ($|V_{j,3}\rangle, |V_{j,4}\rangle, ..., |V_{j,k}\rangle$), the orthogonality constraint increases due to the required orthogonality to all vertex states:

$$\begin{aligned} \langle V_{j,1}|V_{j,k}\rangle &= 0 \\ \langle V_{j,2}|V_{j,k}\rangle &= 0 \\ &\vdots \\ \langle V_{j,k-1}|V_{j,k}\rangle &= 0 \end{aligned} \tag{182}$$

One sees that the arrangements of the phases α_{i_k} for the $|V_{jk}\rangle$-th vertex state depends on $k-1$ constraints:

$$|V_{j,k}\rangle = \sum_{\tilde{j}=0}^{n} \sigma_x^{\otimes\tilde{j}} \otimes \mathbb{1}^{\otimes n-\tilde{j}} \alpha_{0_k}(|V_{j1}\rangle, |V_{j2}\rangle, ... |V_{jk-1}\rangle) \Big| \underbrace{10...0}_{n} \Big\rangle + \alpha_{1_k}(|V_{j1}\rangle, |V_{j2}\rangle, ... |V_{jk-1}\rangle) |010...0\rangle + ...$$
$$+ \alpha_{(n-1)_k}(|V_{j1}\rangle, |V_{j2}\rangle, ... |V_{jk-1}\rangle) |000...1\rangle, \quad \text{with} \quad j = \tilde{j} \quad \text{for} \quad j \leq \left\lfloor \frac{2^n}{n} \right\rfloor, \qquad (183)$$

with $\alpha_{1_k}(|V_{j1}\rangle, |V_{j2}\rangle, ... |V_{jk-1}\rangle)$ being the phase arrangement depending on all phase combinations of the previously constructed vertex states.
Before investigating special cases of bi-, tri- and four partite case a short repetition of the construction of this multiqubit W_k-state simplex may be useful as well as some notable remarks shall be mentioned.

The construction of the W_k-simplex vertex states:

- The canonical W-state is taken as the first vertex state $|V_0\rangle$ comprising n elements of the set of basis states $\mathcal{Z}$, with n being the number of qubits.
- The second orthogonal vertex state $|V_1\rangle$ is created by flipping the first subsystems of $|V_0\rangle$.
- The third vertex state $|V_2\rangle$ is constructed by flipping all subsystems of the second state $|V_1\rangle$.
- This process is repeated until all subsystems have been flipped once.
- Further vertex states are obtained by inverting the existing states. Inverting means here exchanging the „0“ ´s by „1“ ´s and vice versa.
- This gives $\left\lfloor \frac{2^n}{n} \right\rfloor$ vertex states, that can be doubled, tripled, etc. by attaching certain phases to the elements of $\mathcal{Z}$, which build the existing vertex states.
- The total number of vertex states is gained by using all possible phase combinations α_{i_k}, with respect to the orthogonality constraint.
- The number of vertex states created by this construction depends on the number of particles or the dimension of the Hilbert space n and the maximal possible phase combinations k. So the total amount of vertex states is $N_{\text{vertex}}(n,k) = \left\lfloor \frac{2^n}{n} \right\rfloor (k+1)$.

Remarks:

- This construction does include the bipartite case itself, which gives the only W_k-simplex whose dimension coincides with the dimension of the whole Hilbert space (see next chapter).
- The first vertex states $|V_k\rangle$, which carry no phases, are obtained by the flipping operator σ_x. Yet other ways of joining the elements of the basis set $\mathcal{Z}$ are possible, which leads to different vertex states and a different simplices. However all these simplices are unitary equivalent as the only differ by a base transformation in the Hilbert space spanned by $\mathcal{Z}$.

➤ The constructed simplex differs from the dimension of the multipartite qubit system. How much difference occurs depends on the one hand on whether the number of particles is a multiple of 2^n on the other hand how the unity circle is divided by the phases α, whereas these two points are also related to each other. For up to 8 particles the dimensions of the simplices are presented in this table.

Particles n	States without phases $\lfloor \frac{2^n}{n} \rfloor$	Phase arrangements k	Dim. simplex / Dim. Hilbert space
2	2	1	4/4
3	2	2	6/8
4	4	2	12/16
5	6	4	30/32
6	10	4	50/64
7	18	6	126/128
8	32	6	224/256

When regarding the number of different phase combinations a certain pattern can be read out. As previously stated, the combination are related to the orthogonality constraint, however there is a geometrical aspect, that is revealed by investigating how the complex unity circle is divided by the phases:

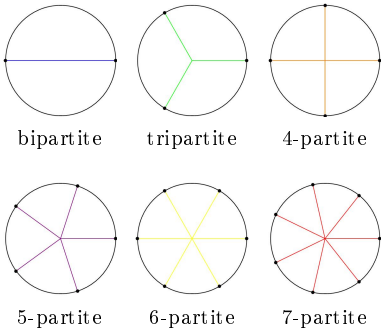


Figure 10: Division of the complex unit circle, $n \leq 7$

For a n-partite qubit system the phases α are represented by n complex numbers lying right on the unit circle in the complex plane (Figure 10). When comparing the division of the unit circle to the number of phase arrangements k a certain pattern arises. The number of phases, that comprise a not vanishing complex part, equals exactly the number of arrangements (except for the bipartite case). The reason for this lies in the symmetry of the phases concerning the real and the complex part, respectively. For an odd dimensional system the symmetry is reduced to the real axis, whereas in the even case it is expanded to the complex axis as well. A higher symmetry, however, reduces the possible phase arrangements. This can be seen by the fact that two phases differ only by a complex conjugation, $Im(\alpha) = Im(\alpha)^*$. This symmetry is also true for the real part of a phase when an even qubit system is investigated, i.e. $Re(\alpha) = -Re(\alpha)$ for n being even. Therefore an odd system leads to more phase arrangements than an even system and also to a higher dimensional simplex, compared to the the number of particles. In the following the simplices are constructed for a given number of particles and investigated by using the previously introduced methods in order to see what kind of geometry is received concerning their entanglement and separability, respectively.

11.2 The bipartite W_k simplex

In this case the exact geometry is known and the previous construction should yield to the very same results. The basis $\mathcal{Z}$ consists of $\Big\{ |00\rangle ; |10\rangle ; |01\rangle ; |11\rangle \Big\}$. The first vertex state,

the W state, that coincides here with the $|\Psi^+\rangle$ state, is constructed by the second and third element of Z, whereas the second vertex state, $|\Phi^+\rangle$, by the remaining two:

$$|V_1\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \quad |V_2\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{184}$$

The phases are $e^{\frac{0\pi i}{2}} = +1$, which is attached on $|10\rangle$, and $e^{\frac{1\pi i}{2}} = -1$, attached to $|11\rangle$:

$$|V_3\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle) \quad |V_4\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \tag{185}$$

As no further phase combinations are possible, the construction leads obviously to the same geometry as it is shown in chapter 9 .

11.3 The tripartite W_k simplex

In this eight dimensional Hilbert space one follows again the previous construction by introducing the set of states $\mathcal{Z}$, the canonical basis:

$$\mathcal{Z} = \Big\{ |000\rangle\,; |100\rangle\,; |010\rangle\,; |001\rangle\,; |110\rangle\,; |101\rangle\,; |011\rangle\,; |111\rangle \Big\}$$

With $\left\lfloor \frac{8}{3} \right\rfloor$ one sees immediately, that two orthogonal vertex states are available and with them a $3 \cdot 2$ dimensional simplex is obtained due to two different phase arrangements. The W state and the resulting flipped state [60] are the first two of the six vertex states :

$$|V_0\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle) \quad V_1 = \frac{1}{\sqrt{3}}(|000\rangle + |110\rangle + |101\rangle) \tag{186}$$

The phases are $\alpha_0 = 1$, $\alpha_1 = e^{\frac{2\pi i}{3}}$ and $\alpha_2 = e^{\frac{4\pi i}{3}}$. In order to receive further vertex states the phases are attached to the elements of the set $\mathcal{Z}$ of the vertex states:

$$|V_{01}\rangle = \frac{1}{\sqrt{3}}(|100\rangle + e^{\frac{2\pi i}{3}}\,|010\rangle + e^{\frac{4\pi i}{3}}\,|001\rangle) \quad V_{11} = \frac{1}{\sqrt{3}}(|000\rangle + e^{\frac{2\pi i}{3}}\,|110\rangle + e^{\frac{4\pi i}{3}}\,|101\rangle) \tag{187}$$

For the last two states, $|V_{02}\rangle$ and $|V_{12}\rangle$, the constraint $\langle V_{01}|V_{02}\rangle = 0$ or $\langle V_{11}|V_{12}\rangle = 0$, respectively, yield the second possible phase arrangement and hence

$$|V_{02}\rangle = \frac{1}{\sqrt{3}}(|100\rangle + e^{\frac{4\pi i}{3}}\,|010\rangle + e^{\frac{2\pi i}{3}}\,|001\rangle) \quad |V_{12}\rangle = \frac{1}{\sqrt{3}}(|000\rangle + e^{\frac{4\pi i}{3}}\,|110\rangle + e^{\frac{2\pi i}{3}}\,|101\rangle). \tag{188}$$

This 6 orthogonal states give the edges of the simplex. In this construction the last two states of the basis set of the $\mathcal{H}^8$ Hilbert space are not part of the vertex states. As stated in the previous chapter the vertex states, and therefore the simplex, could have been composed differently, e.g. by using $1 \otimes \sigma_x \otimes 1$, $1 \otimes 1 \otimes \sigma_x$, $\sigma_x \otimes \sigma_x \otimes 1$, etc. . This would lead to the exclusion of two other basis vectors, but as the vertex states are all unitary equivalent the simplex would have the same geometry.

[60] Here the flip operator $\sigma_x \otimes 1 \otimes 1$ is applied.

Also a phase space structure can be drawn (see Figure 11), in which the dots represent the six vertex states, that differ either by flipping (horizontal axis) or by phase shifting (vertical axis) or by both. In order to investigate the simplex, different states are determined, which consist of weighted superpositions of vertex states. In this work two different weights are used, because of the possibility to find symmetries and geometrical properties in a two dimensional picture, which is mathematically a projection of the whole simplex onto a two dimensional plane.

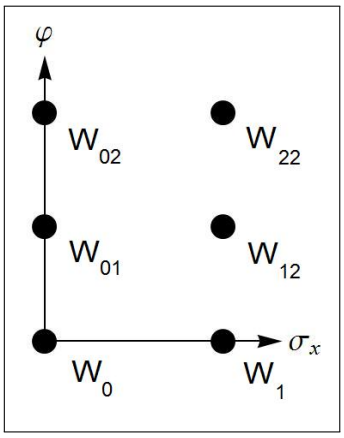
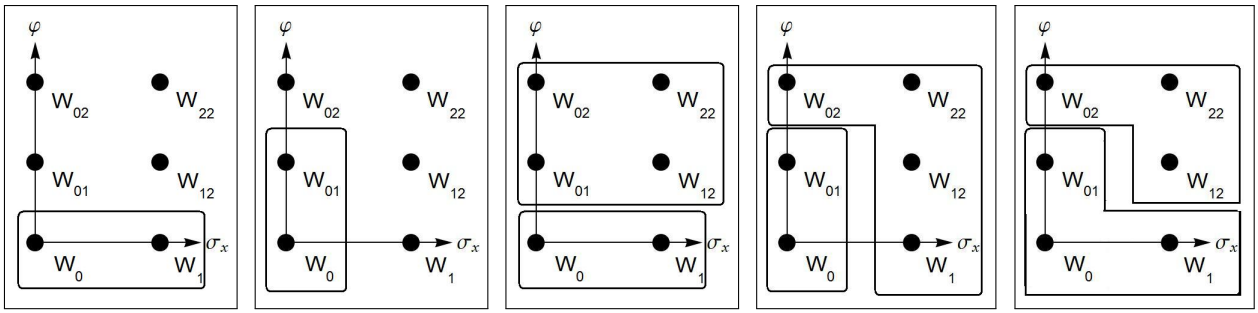


Figure 11: Phase space of the three qubit case

This means in general that a an arbitrary state of a two dimensional projection of this simplex is given by $|S\rangle\langle S| = a \sum_k W_k + b \sum_l W_l + (\frac{1-a-b}{6}) \sum_{m\neq k,\neq l} W_m$, with k, l, m being elements of an index set and $W_i := |V_i\rangle\langle V_i|$, with $i \in \{0, 01, 02, 1, 11, 12\}$.
It turns out that all two parameter states of the simplex can be classified into five equivalence classes, whereas within every class the same results are found concerning positivity, partial transposition, realignment and application of the entanglement measure.

The five equivalence classes are given by this combination of states:



1st group 2nd group 3rd group 4th group 5th group

Figure 12: Equivalence classes of the 3 dim. W_k-simplex

Figure 12 only shows one representative of each class, as for example the first group of states ρ_1 contains two vertex states from one row, i.e. these states are the weighted superposition of two vertex states, that differ by a flip operation, in this example $\rho = a\, W_0 + b\, W_1 + (\frac{1-a-b}{6}) \sum_{m\neq 0\neq 1} W_m$.
It turns out that for all classes of states only entangled states can be found within every two dimensional projection, which allows to deduce that this whole six dimensional simplex consists of entangled states. This is due to the missing two dimensions in comparison to the whole Hilbert space, as one will see in later. This means further that with the given vertex states no separable states can be constructed, that can be represented in a geometrical picture. However by allowing a mixture of this classes with the maximally mixed state $\mathbb{1}$, the properties of the classes of states hence change, as by that the two missing dimensions are added.

Therefore the class of states under investigation are then given by

$$|S\rangle\langle S| = a \sum_k W_k + b \sum_l W_l + (\frac{1-a-b}{6})\ \mathbb{1}, \tag{189}$$

with $W_{k/l}$ being the previously denoted a vertex state. Via this 'cheating' the five class of states remain and a more interesting simplex is gained, as the different classes are regarded.

First class of states

The first class of states can be stated in the form

$$\rho_1(a,b) = aW_{\text{left}} + bW_{\text{right}} + \frac{1-(a+b)}{8}\mathbb{1}, \tag{190}$$

with $\left|V_{\text{left/right}}\right\rangle$ being a state of the left/right column. Applying now different criteria, as they were introduced in the previous sections the following results are obtained.

Positivity

The positivity of the first class states, $\rho_1 > 0$, depends on the weights (a, b) and leads to the triangle embedding all states, as shown in Figure 13

PT-criterion

The partial transpose operation leads to positive eigenvalues for certain weights, i.e. to separable states bounded in region **I**. As it is shown in chapter 4, the partial transposition is constructed for bipartite systems. However it also provides results for more qubit cases, as every state can be seen as a combination of a bipartite state when a certain cut is introduced, dividing the state into two parts (see chapter 2.2). That means that for these tripartite states the combinations 1|23, 12|3,13|2 have to be considered, with 1,2 and 3 denoting the subsystem of one qubit. The constructed bipartite state is hence an element of the Hilbert space, $\mathcal{H}^2 \otimes \mathcal{H}^4$. According to this separation three different partial transposed matrices are received. Due to the high symmetry of this class of states all transposed matrices lead to the same positivity and therefore to the same region. It is obvious that via this approach only bipartite entanglement can be detected.

Entanglement measure

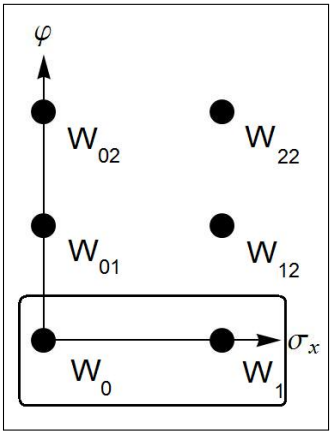
The entanglement measure is detecting no entanglement in region **II**. That means on the other hand that entangled states are found outside this region. It also has to noted that entanglement between each combination of the two subsystems as well as three particle entanglement is found in the same proportion. It can also be recognized that the detection of the partial transposition is more exact for this case compared to the entanglement measure, which obviously depends from the numerical bounds. It will turn out that this difference in detection also depends on the states itself. It also has to be noted that the entanglement measure is calculated numerically.

Realignment criteria

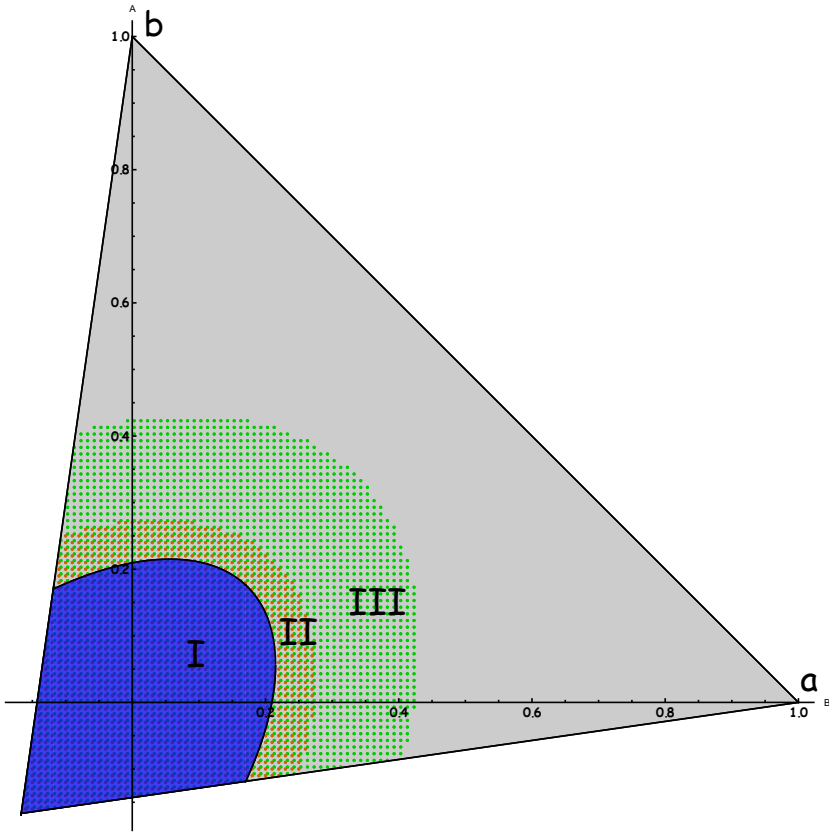
This criterion is just like the partial transposition, constructed for bipartite systems. When following the same argument as used in the partial transposition case. also three different

cases have to be considered, that coincide again due to the high symmetry. In Figure 13 it is given by the third region (**III**). Also for the realignment criteria a numerical method is used. However the accuracy of discrimination between separable and entangled states is the lowest, compared to the first two.

It also has to be noted that this class is completely symmetric according to the parameters a and b. The whole geometry of this first class of states is shown in following figure:



1st group



Geometry of the 1st class

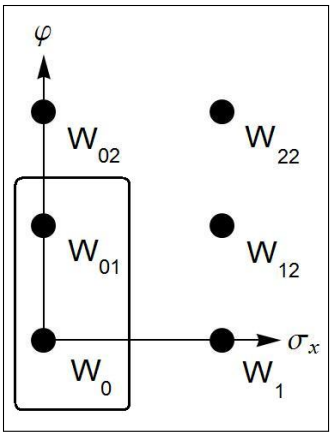
Figure 13: Geometry of the first equivalence class of states

Second class of states

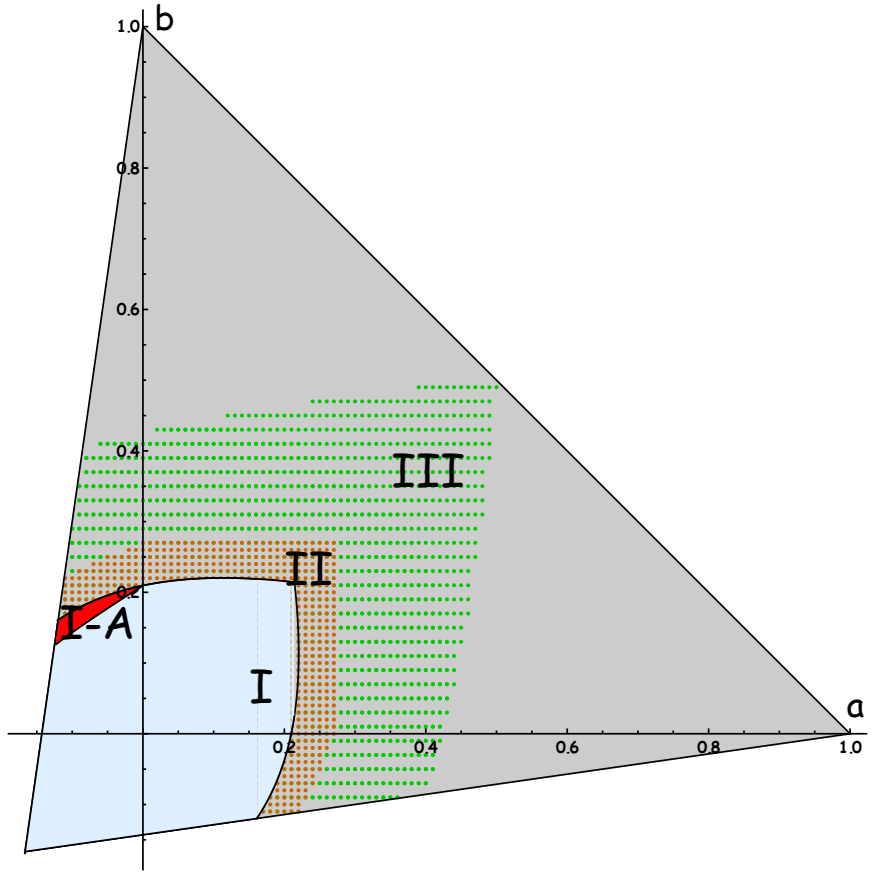
The states of the second class are of the form

$$\rho_2(a,b) = a\ W_{\text{left/right}} + b\ W_{\text{left/right}} + \frac{1-(a+b)}{8}\mathbb{1}, \tag{191}$$

whereas two, but not the same two states of one column are taken for the superposition. Regarding again the same properties as in the previous class, it can be seen (Figure 14), that, beside the same positivity, a similar region of positive partial transposition (**I**) as well as a similar amount of separability is found by the entanglement measure (**II**). Again the realignment criterion (**III**) is detecting the fewest states compared to the other two. Another notable phenomena that occurs in this class of states is given by the partial transposition. The partial transposition is unlike in the previous case not completely symmetrical for the transposition of the subsystem. The red region (**I-A**) indicated a small area that denotes negative eigenvalues for states that are transposed with respect to the 1|23 cut, i.e transposition of the first subsystem.



2nd group



Geometry of the 2nd class

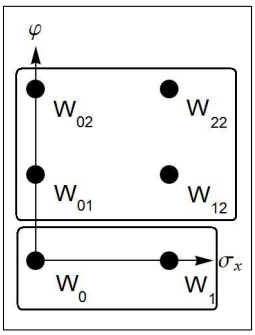
Figure 14: Geometry of the second equivalence class of states

Third class of states

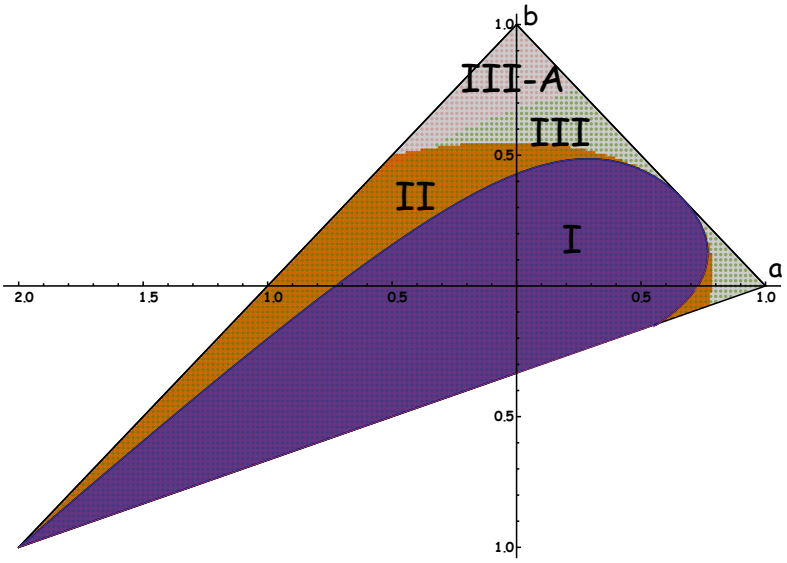
The third class comprises states that consist of the superposition of a vertex state of the left and the right column with the remaining four vertex states and the maximally mixed state, i.e.

$$\rho_3(a,b) = \frac{a}{2}(W_{\text{left/right}} + W_{\text{right/right}}) + \frac{b}{4}(W_{\text{left}} + W_{\text{left}} + W_{\text{right}} + W_{\text{right}}) + \frac{1-(a+b)}{8}\mathbb{1}. \tag{192}$$

These states already differ from the previous one by their positivity, as the left edge of the triangle is enlarged to the $(-2, 1)$ point. Also a larger area of separable states is obtained by all criteria. A remarkable difference compared to the latter cases is that the bounds of the entanglement measure (**II**) are close or even equal to the partial transposition criteria (**I**), which differs again for the transposition of the first subsystem, marked by the (**I-A**) region. On the other hand it can be seen that the area resulting from the realignment criteria is hardly detecting any entanglement, as it can all be seen in Figure 15



3rd group



Geometry of the 3rd class

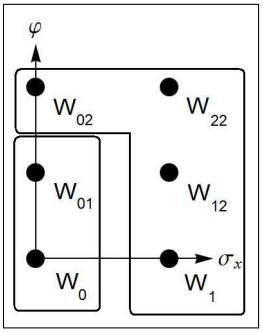
Figure 15: Geometry of the third equivalence class of states

Fourth class of states

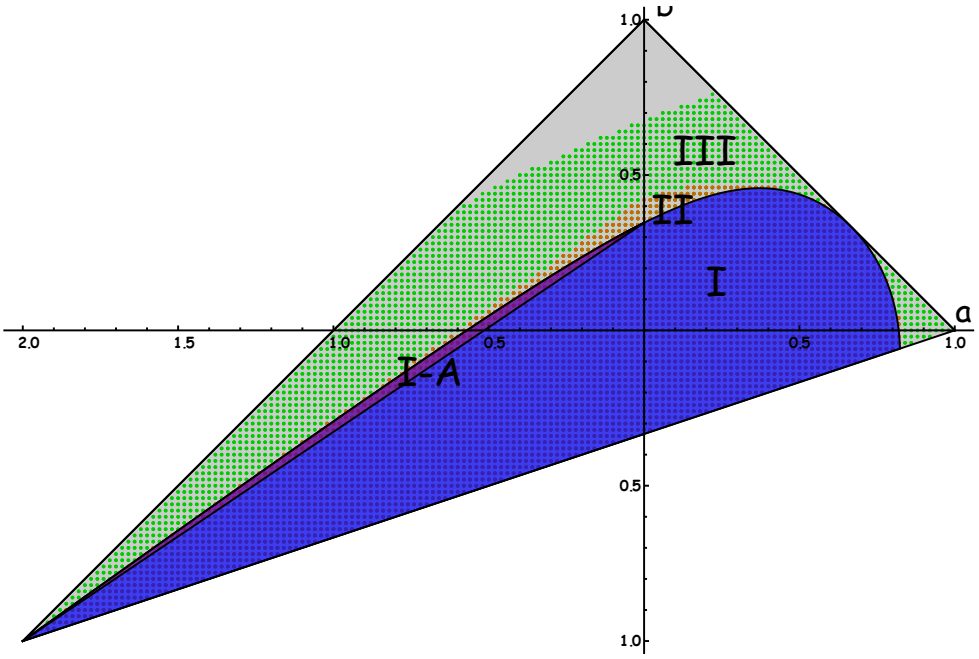
Similar to the third class the fourth class of states is given by the superposition of two vertex states of one column with the remaining five vertex states (three from one column and one from the other) and the maximally mixed state, i.e.

$$\rho_4(a,b) = \frac{a}{2}(W_{\text{left/right}} + W_{\text{left/right}}) + \frac{b}{4}(W_{\text{left}} + W_{\text{right/left}} + W_{\text{right/left}} + W_{\text{right}}) + \frac{1-(a+b)}{8}\mathbb{1}. \tag{193}$$

As the states are constructed similar to the latter equivalence class the resulting geometry is also very similar. The lower bounds of the entanglement measure (**II**) are in this case even closer to the positive partial transposition (**I**), while again the singular values of the realigned matrix that are smaller than 1 give the third (**III**) bound.



4th group



Geometry of the 4th class

Figure 16: Geometry of the fourth equivalence class of states

Fifth class of states

With the fifth equivalence class the remaining possible combinations of states with two parameters is given. The states are comprising the superposition of two vertex states of one and one vertex state of the other column, combined with the remaining three states and the Identity. This means written in the density formalism,

$$\rho_4(a,b) = \frac{a}{3}(W_{\text{left/right}} + W_{\text{left/right}} + W_{\text{right/left}}) + \frac{b}{3}(W_{\text{right/left}} + W_{\text{right/left}} + W_{\text{left/right}}) + \frac{1-(a+b)}{8}\mathbb{1}. \tag{194}$$

The geometrical picture of this class is shown in the following picture.

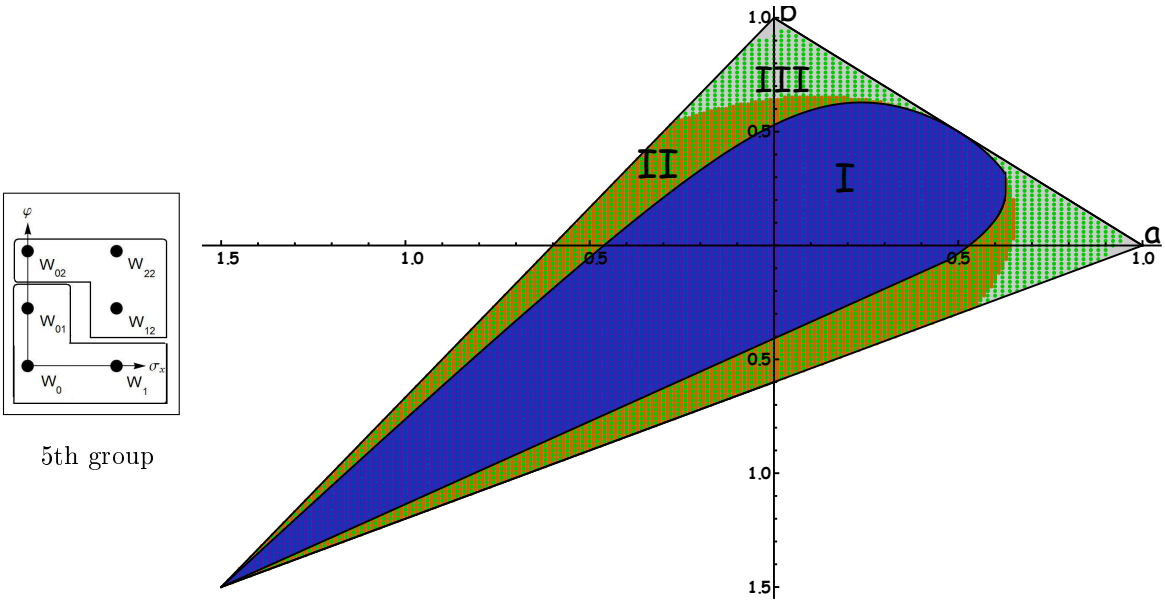


Figure 17: Geometry of the fifth equivalence class of states

As one can see the geometry of this class is similar to the latter two classes, again with the blue area (**I**) being the positive partial transpose, the orange region denoting the lower bounds of the entanglement measure (**II**) and the green border giving the numerical results of the realignment criteria (**III**)

11.4 The Second Construction

Another alternative construction of a W_k state simplices is given by using the W basis that was introduced by Briegl et al. for the case of multipartite distillation. As already stated in chapter 6.2 this construction uses the stabilizer formalism which allows to write the vertex sates of a n particle W_k state simplex as the W basis states. Therefor the vertex states are constructed by applying the operator U_W to all n elements z_i of the set of the canonical basis $\mathcal{Z}$, i.e. the i-th vertex state is given by

$$|W_{z_i}\rangle := U_W \, |z_i\rangle \,, \tag{195}$$

with $U_W = \frac{1}{\sqrt{n}} \sum_{l=1}^{n} \sigma_z^1 \otimes \sigma_z^2 ... \otimes \sigma_z^{l-1} \otimes \sigma_x^l \otimes \mathbb{1}^{l+1} \otimes \mathbb{1}^{l+2} ... \otimes \mathbb{1}^n$ containing the stabilizer operators. The table, written on page 43 shows the three dimensional case of this basis explicitly. From the geometrical point of view a higher symmetry of this simplex is found, since for simplex cuts, similar to the previous choice, only two possibilities occur. Contrary to the previous construction no phase space digram can be established as the distribution into state flips by the σ_x operator as well as the phase shifts are of a more complex form. However another symmetry can be posed, when investigating the convex weighted sum of two vertex states with the maximally mixed state, the identity. Using the notation of section 6.2 every vector state can be uniquely addressed by a binary number. E.g. in the three qubit case the first vector, the W-state is given by '000', the second by '001' and so on. When using again the inverse operator $\mathcal{I}$ that switches the '0' to '1' and the '1' to '0', respectively, the geometry of a state $\rho = a \ |W_{z_i}\rangle + b \ \left|W_{z_j}\right\rangle + \mathbb{1}_n$ is equal to its inverted $\rho^I = a \, \mathcal{I}(|W_{z_i}\rangle) + b \, \mathcal{I}(\left|W_{z_j}\right\rangle) + \mathbb{1}_n$ with respect to the applied criteria, i.e. the partial transposition as well as introduced multipartite measure.
As an example for this statement states are investigated that are given by the superposition of two different W basis states and the mixture of the remaining six. As in the previous simplex different classes of states can be determined. The following states are representatives of the three different classes of states:

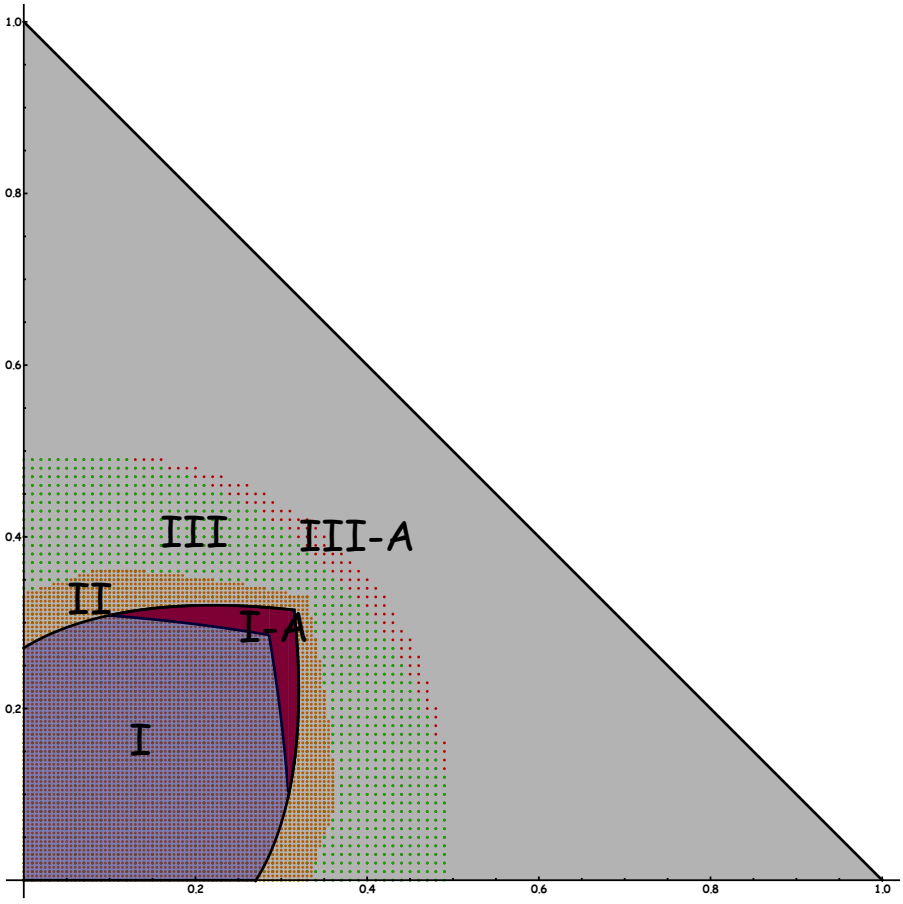
$$\rho_1 := a \ |000\rangle\langle 000| + b \ |001\rangle\langle 001| + \frac{1-a-b}{6} \ |\text{remaining states}\rangle$$
$$\rho_2 := a \ |000\rangle\langle 000| + b \ |011\rangle\langle 011| + \frac{1-a-b}{6} \ |\text{remaining states}\rangle$$
$$\rho_3 := a \ |000\rangle\langle 000| + b \ |111\rangle\langle 111| + \frac{1-a-b}{6} \ |\text{remaining states}\rangle$$

As it turns out, states of this form can be classified by their amount of excited substates, i.e. ρ_1 represents states with one excited substate, as it contains one 1, ρ_2 the class of states with two excited subsystems and so on. States with four to six excited subsystems are underlaying the same geometry as they can be lead back to the classes with one to three excited subsystems by applying the inverse operator I. Therefore it is sufficient to investigate one of the representatives of the three classes in order to determine its geometry according to the above stated criteria.

First class of states

For ρ_1 the geometry is given in Figure 18. As previously, marked spaces determine separable states, each received by different methods. The first region (I) is determined by the partial transposition, whereas it has to be noted that, due to the symmetry of the states,

the partial transposition of one subsystem leads to a different bound, indicated by the red area (I-A). Which of the transposed subsystems leads to this symmetry breaking depends on the subsystem that is in the excited state 1. The second area (II) shows the lower bounds of the multipartite entanglement measure, which also determines, that the states outside this area are three partite as well as two partite entangled. Furthermore the third region (III) is received by the realignment criteria, which has to be distinguished whether the realignment of this three qubit state is done via two dimensional (III-A) or four dimensional submatrices (III). For this as well as for the following two classes of states the geometry of the states is symmetrical concerning the exchange of the parameters a and b.

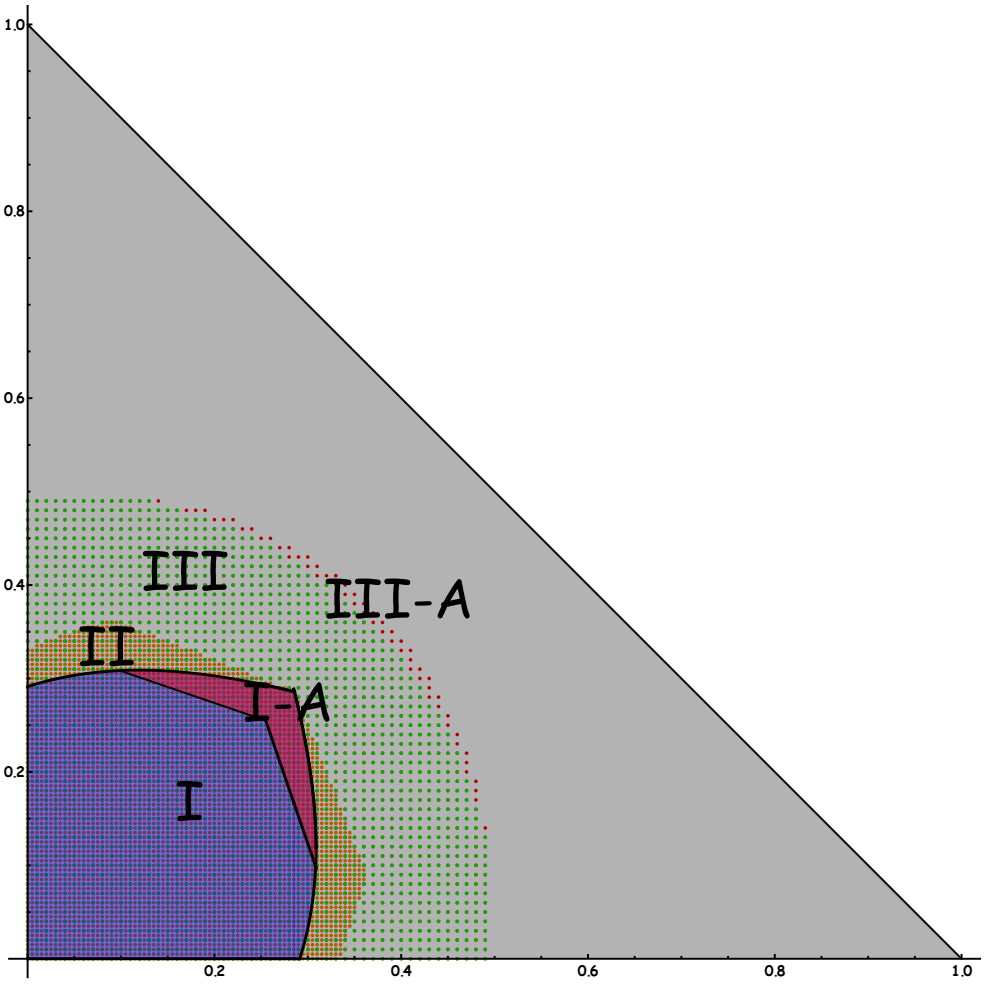


Geometry of the 1st class

Figure 18: Geometry of the first class of states

Second class of states

Also for states with two excited subsystems, as for example ρ_2 the geometry is very similar to the latter case, as the regions occur in almost the same way, again with the broken symmetries for the partial transposition as well as for the realigned matrices. Figure 19 shows the different regions.

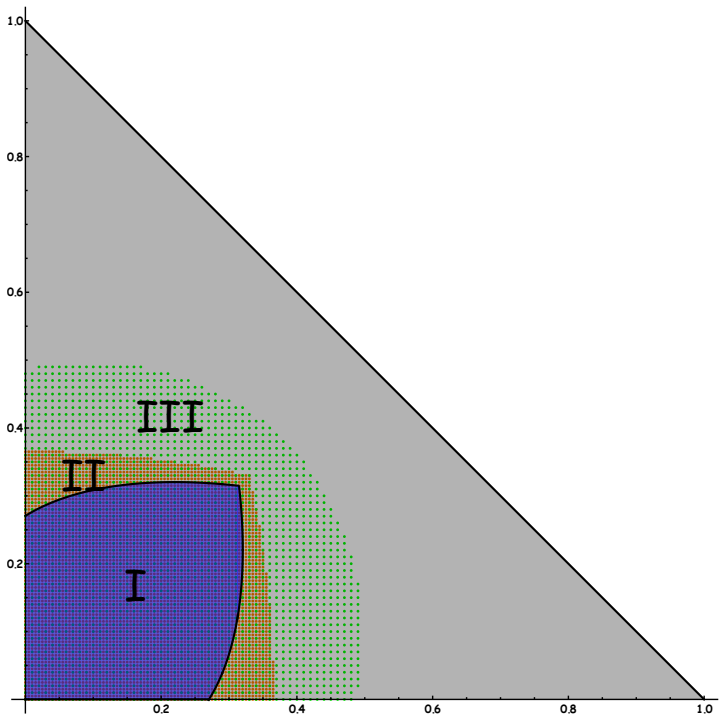


Geometry of the 2nd class

Figure 19: Geometry of the 2nd class of states

Third class of states

The states with three excited subsystems show the highest symmetry of the three classes. This leads to the same partial transposed state regardless on which of the subsystem the transposition is applied. Also the realignment of the states according to two and four dimensional submatrices lead to the same boundary. Figure 20 shows the geometry of the this class.

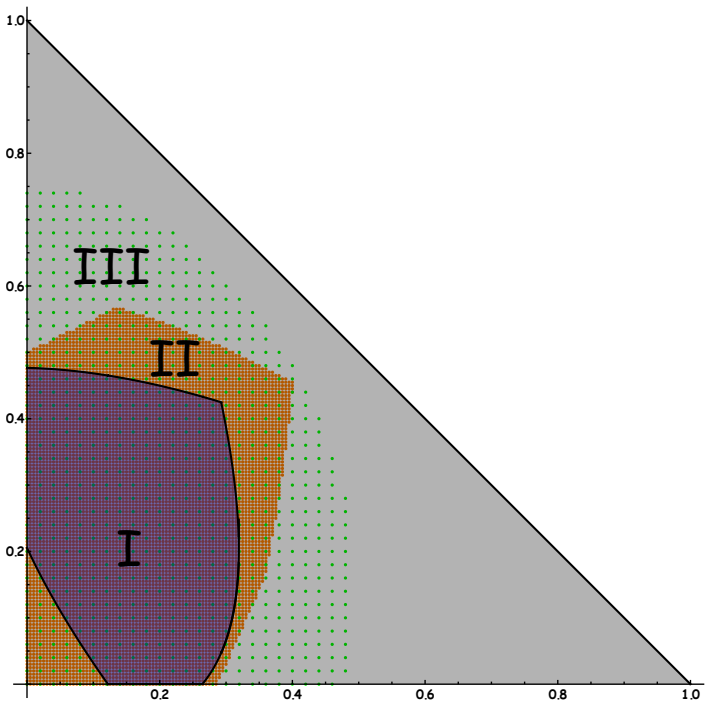


Geometry of the 1st class of states

Figure 20: Geometry of the first equivalence class of states

Other than the previous construction in section 4.3 no phase space structure is established, as mentioned before. However beside these combinations of two states different combinations of W-basis state lead to a more complex geometry. As an example Figure 21 shows the geometry of the state

$$\rho_1 := \frac{a}{2}\left(|000\rangle\langle 000| + |011\rangle\langle 011|\right) + \frac{b}{2}\left(|001\rangle\langle 001| + |010\rangle\langle 010|\right) + \frac{1-a-b}{4}\left(|100\rangle\langle 100| + |110\rangle\langle 110| + |101\rangle\langle 101| + |111\rangle\langle 111|\right). \tag{196}$$



Geometry of the 1st class of states

Figure 21: Geometry of the first equivalence class of states

For this case the partial transposition criterion is detecting entanglement also in the region around $a = b = 0$, whereas the area of separable states (I) is shifted compared to the previous states. However this difference is undetected by the entanglement measure (II) as well as by the realignment criterion (III).

CHAPTER 12

Magic Simplex

The Magic Simplex represents another generalization, namely the expansion to three and more degrees of freedom within a bipartite quantum system, first shown in [74, 12]. This means contrary to the previous chapters, the retention of two particles, each with d degrees of freedom, and a $\mathcal{H}^d \otimes \mathcal{H}^d$ dimensional Hilbert space. Therefore the situation in terms of maximally entangled states simplifies, as they can be constructed uniquely. Similar to the multiparticle cases these states denote the orthogonal vertices of the Magic Simplex.
The construction in detail starts with the state $\Omega_{0,0} := \sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle$, the first pure, maximally entangled vertex state of a $\mathcal{H}^{d^2}$ Hilbert space. Further vertex states are obtained by applying d^2 different Weyl-operators $W_{k,l}$ (see equations (21), (22)) on one of the two subsystems of the existing state $\Omega_{0,0}$ (here w.l.o.g on the first subsystem):

$$\begin{aligned} |\Omega_{k,l}\rangle &:= W_{k,l} \otimes \mathbb{1} \quad \sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle \\ |\Omega_{k,l}\rangle &:= e^{\frac{2\pi}{d} l(i-k)} \quad \sum_{i=0}^{d-1} |i-k\rangle \otimes |i\rangle \end{aligned} \tag{197}$$

With $k, l \in k, l \in \{0, 1, ..., d-1\}$ the Magic Simplex is given by the convex sum of d^2 projectors $P_{k,l}$, which are the density matrices of $\Omega_{k,l}$´s, $P_{k,l} = |\Omega_{k,l}\rangle \langle\Omega_{k,l}|$. They project on the subspaces spanned by all vertex states,

$$\mathcal{W} \quad = \quad \Big\{ \sum c_{k,l} P_{k,l} \mid c_{k,l} \geq 0, \quad \sum c_{k,l} = 1 \Big\}. \tag{198}$$

Geometrically the Magic Simplex $\mathcal{W}$ is, due to the constraints on the coefficients $c_{k,l}$, a d^2-1 dimensional hyperplane of a d^2 dimensional Euclidean space $\{A = \sum a_{k,l} P_{k,l} \mid a_{k,l} \in \mathbb{R}\}$. On this Euclidean space a distance relation $\sqrt{Tr(A-B)^2}$ with the associated norm $\sqrt{A^2}$, which is called the Hilbert-Schmidt Norm, as well as an inner product $Tr(AB) = \sum a_{k,l} b_{k,l}$ can be established.
A further notable point is that the Magic Simplex contains by construction only locally maximally mixed states. However it can be shown that $\mathcal{W}$ is just a subspace of the set of all maximally mixed states, as the existence of maximally mixed states outside the simplex can be proven [74, 12].
The most important property of $\mathcal{W}$ is the high symmetry of the states included in $\mathcal{W}$.
For the sake of simplicity the following results are true for the 9 dimensional Hilbert space, i.e. bipartite qutrits are investigated, but all results can be generalized to higher dimensional degrees of freedom:
It can be shown that all unitary transformations of states inside the Magic Simplex have its counterpart in this phase space, e.g. a vertical shear in the phase space is given by the operator $\mathcal{V}$, that cases an index shift on the first index of $P_{k,l} \to P_{k+l,l}$. This fact can be illustrated in a Phase space diagram (Figure 22) with each point referring to a $P_{k,l}$:

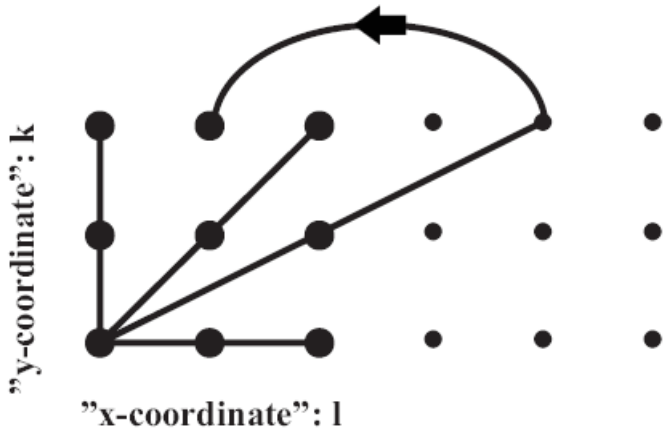


Figure 22: Phase space diagram of the Magic Simplex

More general the following theorem can be stated:
Theorem:
The group of symmetry transformations in the Magic Simplex $\mathcal{W}$ is equivalent to the group of affine index transformations in the phase space,

$$\begin{pmatrix} k \\ l \end{pmatrix} \to \begin{pmatrix} m & n \\ p & q \end{pmatrix} \begin{pmatrix} k \\ l \end{pmatrix} + \begin{pmatrix} j \\ r \end{pmatrix},$$

with $mq - pn \neq 0$ and with all indices being integers modulo 3. Note that for $mq - pn = \pm 1$ the transformations of the Hilbert space is unitary and anti-unitary, respectively.

Another theorem can be proven using the symmetry and the transformation equivalence of this phase space representation:

Theorem:
When investigating the classes of subsets of phase space points it turns out that all subsets containing a single point are equivalent. The same is true for a pair of points. For a triple or a quadruple combinations of points there exist two equivalence classes each. Combinations of 5-8 points are part of one of the complementary sets of these 6 equivalence classes as the counterparts of the 1-4 combinations in this 9 dimensional phase space. It can be shown further that permuting points pair- or triple wise has no effect, as there is total symmetry under permutations.

With these symmetries in mind the geometry of the simplex concerning separability and entanglement can be shown. The tools are the following:

- **Polytopes**
  An obviously separable state of the simplex is given by the maximally mixed state $\frac{1}{9}\mathbb{1}$, which can be written as the equally weighted superposition of all vertex states $P_{k,l}$, $\frac{1}{9}\mathbb{1} = \frac{1}{9}\sum_{k,l} P_{k,l}$. Considering now the states with the larges possible distance from this state, which are still separable. When these states are used to create hyperplanes comprising these states a polytope is build, which gives an outer fence for all separable states, as the used states had the maximal distance to maximally mixed states. These states can be shown to have the form, $\rho_{line} := \frac{1}{3}\sum_{(k,l)\in line} P_{k,l}$, whereas the indices k, l

are restricted by a line of the phase space diagram. Because of the unitary equivalence of point of the phase space each of this lines has three equivalence sets [61], which leads to 12 outermost states ρ_{line}.
Then the hyperplanes are given by $B_{p,q} = \left\{(c_{k,l})|c_{p,q} = \frac{1}{3}\right\}$ and $A_{p,q} = \{(c_{k,l})|c_{p,q} = 0\}$. Combined to the outer fence, the enclosure polytope is given as

$$\left\{(c_{k,l})| \quad \text{all} \quad c_{p,q} \in \left[0, \frac{1}{3}\right]\right\}. \tag{199}$$

Using the ρ_{line} states in a similar way, but combining the hyperplanes in a different way by using the different intersections of the hyperplanes an inner fence can be posed as well, which is called the kernel polytope

$$\left\{\rho = \sum_{lines\alpha} \lambda_\alpha \rho_{line\alpha} | \lambda_\alpha \geq 0, \sum \lambda_\alpha = 1\right\} \tag{200}$$

➤ **Partial Transposition**
Basically the task here is given by applying the partial transposition on a $9x9$ matrix and determine whether the resulting matrix is positive or negative. But as the matrices of the Magic Simplex are build in a special way, a more elegant and easier method can be introduced. As the basis vectors are given by $|s-l, s\rangle = |s-l\rangle \otimes |s\rangle$ the resulting density matrices can be ordered in groups of three, according to l, and inside each l according to s. Therefore the entire Hilbert space can be split up into the direct sum of these indices

$$\mathcal{H}^3_{l=0} \oplus \mathcal{H}^3_{l=1} \oplus \mathcal{H}^3_{l=2}. \tag{201}$$

Also for the states these splitting is valid and an arbitrary density matrix inside the simplex can be expressed by using the introduced Projectors $P_{k,l}$ as

$$\rho = \sum_{k,l} c_{k,l} P_{k,l} = (\sum_k c_{k,0} P_k) \oplus (\sum_k c_{k,1} P_k) \oplus (\sum_k c_{k,2} P_k), \tag{202}$$

with $P_0 = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, P_1 = \frac{1}{3}\begin{pmatrix} 1 & \omega^* & \omega \\ \omega & 1 & \omega^* \\ \omega^* & \omega & 1 \end{pmatrix}$ and $P_2 = \frac{1}{3}\begin{pmatrix} 1 & \omega & \omega^* \\ \omega^* & 1 & \omega \\ \omega & \omega^* & 1 \end{pmatrix}$.
Or even more general in the present case for all states inside of the 9 dimensional simplex $A_{l=0} \oplus A_{l=1} \oplus A_{l=3}$ a representation with the matrix

$$A = \frac{1}{3}\begin{pmatrix} d & a^* & a \\ a & d & a^* \\ a^* & a & d \end{pmatrix}, \quad d_l = \sum_k c_{k,l}, \quad a_l = \sum_k \omega^k c_{k,l} \tag{203}$$

is possible. As it is proved in [12] the partial transposition of states inside $\mathcal{W}$ reorders the elements of the matrix A to a new matrix

$$B = \frac{1}{3}\begin{pmatrix} d_0 & a_2 & a_1^* \\ a_2* & d_1 & a_0^* \\ a_1 & a_0 & d_2 \end{pmatrix}. \tag{204}$$

[61] The the horizontal line on the bottom is the same as the horizontal line using the three middle or top points, respectively.

The positivity of B leads to constraints on the coefficients $c_{k,l}$ and the regions of PPT, NPT, respectively, as well as to the prospective regions of separability and entanglement. It has to be reminded that the partial transpose criteria is no longer sufficient in this case.

➤ **Entanglement Witnesses**
Similar to the witnesses, introduced in chapter 8, a set of operators is defined, which act as two different types of witnesses. The structural witness (SW) is a convex set of operators, that are defined by the action on a separable state σ:

$$SW := \left\{K = K^\dagger \neq 0 | \forall \sigma \in SEP : Tr(\sigma K) \geq 0\right\} \tag{205}$$

A subset of this definition is useful as it responds with the surface of this set and therefore with the surface of the set of separable states. This subset is called the tangential witness (TW) and can be posed by the action of an operator on a separable state σ as well as on state ρ that is on the surface of SEP,

$$TW_\rho := \left\{K = K^\dagger \neq 0 | \forall \sigma \in SEP : Tr(\sigma K) \geq 0, Tr(\rho K) = 0\right\} \tag{206}$$

The symmetries of the Magic Simplex and the connection to the phase space structure is formulated in the following Theorem:
Theorem:
For a density matrix ρ that is invariant under elements V_g of a symmetry group $\mathbb{G}$ [62], $V_g \rho V_g^{-1} = \rho$, these propositions hold:

I If ρ is entangled $\Rightarrow \exists \quad EW_\rho$, that is $\mathbb{G}$-invariant

II If ρ is on the surface of SEP $\Rightarrow \exists \quad TW_\rho$, that is $\mathbb{G}$-invariant

III The subset of SEP comprising all $\mathbb{G}$-invariant density matrices is completely characterized by the set of $\mathbb{G}$-invariant TW_ρ

IV The previous results hold also for all ρ being elements of the PPT-set

Regarding these results with the group of unitary operators, namely $U_{k,l} = 2P_{k,l} - \mathbb{1}$ and products of it, the corresponding witness $K = \sum_{k,l} \kappa_{k,l} P_{k,l}$ is exactly the operator that has to be chosen in order to determine the SEP and the set of PPT states, as all $P_{k,l}$ and its linear span, the simplex $\mathcal{W}$, are point wise invariant under $U_{k,l}$. Based on this operators a further relation is found:
Theorem:
The operator

$$K = \sum_{k,l} \kappa_{k,l} P_{k,l} \tag{207}$$

is a structural witness for a state $\rho \in \mathcal{W}$ iff the operator

$$M_\Phi = \sum_{k,l} \kappa_{k,l} W_{k,l} \left|\Phi\right\rangle \left\langle\Phi\right| W_{k,l}^{-1} \quad \forall \Phi \in \mathcal{H}^3 \tag{208}$$

is not negative. Iff $\exists \Phi$ such that $\det M_\Phi = 0$ K is even a TW.

[62] This symmetry group consists of unitary and/or anti-unitary operators, which represent shifts and reflections inside the phase space structure.

This theorem claims that every witness operator $K \in \mathcal{H}^9$ is connected to a set of operators $M_\Phi \in \mathcal{H}^3$, whereas the more habile $M_\Phi s$ can be used to calculate the TW and the borders of SEP and PPT, respectively. As a possible application of this theorem one can consider states that are located on one of the three lines. W.l.o.g.[63] the bottom line of the phase space points is taken, which is invariant under these unitary operators $\sum_s e^{i\delta(s)} |s\rangle \langle s|$ (compare Weyl-operators $W_{k,0}$). Also adding the unity does not change this symmetry. Hence the corresponding witness for those states is given by

$$K = \lambda \frac{1}{3} \mathbb{1} + \sum_k \gamma_k P_{k,0} \tag{209}$$

and referring to the previous theorem the operator M_Φ

$$M_\Phi = \lambda \frac{1}{3} \mathbb{1} + \sum_{k=0}^{2} \gamma_k P_{k,0}. \tag{210}$$

According to the theorem a state on the surface of SEP can be found by a TW, which is characterized by $det M_\Phi = 0$, here

$$\begin{aligned} \det M_\Phi = \lambda^3 &+ \|\Phi\|^2 (\gamma_0 + \gamma_1 + \gamma_2)\lambda^2 \\ &+ 3(|\Phi_0|^2 |\Phi_1|^2 + |\Phi_1|^2 |\Phi_2|^2 + |\Phi_2|^2 |\Phi_0|^2)(\gamma_0\gamma_1 + \gamma_1\gamma_2 + \gamma_2\gamma_0)\lambda \\ &+ 27 |\Phi_0|^2 |\Phi_1|^2 |\Phi_2|^2 \gamma_0\gamma_1\gamma_2 \end{aligned} \tag{211}$$

Further investigation of this polynomial leads to four different types of witnesses, specified by the variables λ, γ_0 and $\gamma = \frac{1}{2}(\gamma_1 + \gamma_2)$. From these operators four vertex states σ_i are received corresponding to the linear regions of the witnesses.

1. $\lambda = 1, \quad \gamma \geq 0, \quad \gamma_0 = -1 \quad \Rightarrow \quad \sigma_1 = \mathbb{1} + \frac{2}{9}P_{0,0} - \frac{1}{9}P_{1,0} - \frac{1}{9}P_{2,0}$
2. $\lambda = 1, \quad 0 \geq \gamma \geq -\frac{2}{3}, \quad \gamma_0 = -1 - 2\gamma \geq \frac{1}{3} \quad \Rightarrow \quad \sigma_2 = \frac{1}{3}(P_{0,0} + \frac{1}{9}P_{1,0} - \frac{1}{9}P_{2,0})$
3. $\lambda = 1, \quad \gamma = -\frac{2}{3}, \quad \gamma_0 \geq \frac{1}{3} \quad \Rightarrow \quad \sigma_3 = \frac{3}{4}(\mathbb{1} - \frac{1}{9}P_{0,0} + \frac{2}{9}P_{1,0} + \frac{2}{9}P_{2,0})$
4. $\lambda = 0, \quad \gamma \geq 0, \quad \gamma_0 = 1 - \gamma > 0 \quad \Rightarrow \quad \sigma_4 = \frac{3}{2}(\mathbb{1} - P_{0,0} + \frac{1}{3}(P_{1,0} + P_{2,0} + P_{3,0}))$

All results and observations, including the entanglement and separability criteria, can be generalized to a bipartite system with an arbitrary degree of freedom [74] due the preponderant analytical calculations. Even the helpful phase space structure is preserved, of course conformed to the degree of freedom with more vertex points. For the $\mathcal{H}^4 \otimes \mathcal{H}^4$ case the region of separability for states in the 16 dimensional Magic Simplex, which are combined by the vertex states of one line, the witness K is given analogue to the 9 dimensional case before (eq. 212) as

$$K = \lambda \frac{1}{4} \mathbb{1} + \sum_{k=0}^{3} \gamma_k P_{k,0}.$$

Due to the Theorem also the corresponding operator M_Φ looks equal, considering that the Unity has to be taken as a 4x4 matrix and the sum running from 0 to 3. Despite of the

[63] All lines are unitary equivalent due to the high symmetry.

hopeful generalization problems arise when it comes to the geometry of a special class of states in higher dimensions. Not only the size of the density matrices increases, which makes the partial transposition to an awkward calculation, but also the witnesses cause problems.

CHAPTER 13

Conclusion and Outlook

As far as one can see from the presented theories and its geometrical illustration, it is obvious that this is only a sketch from the great amount of results that have been found and also will be in this theory of quantum mechanics. Due to the fact that we all are more or less visual human beings these graphics may help to get another helpful perspective on the rather puzzling and uninspiring mathematical theory. The only drawback of this visualization, as already stated before, occurs when either more particles or more degrees of freedom are taken into account, as the presented criteria are based on matrix analysis, which is, even in the numerical case, hard to handle with the present programs. However from the lower dimensional cases also a lot can be learned. For example the fact that the different equivalence classes of states, which are combined in different simplices, and their individual geometry are reflecting the assumption that all introduced criteria are somehow connected. Not only the fact that mostly every entanglement criteria presented in this thesis can be deduced in more than way but also the peculiar point that the geometrical boarders of the different criteria are similarly shaped or even equal for the different classes of state, gives rise to this conjecture. Furthermore many exciting problems, like the existence of NPT bound entangled states or even the behavior of entanglement under relativistic terms, are still open. Hence on a more fundamental level, namely whether quantum mechanics is the right choice of describing these problem, and even if this is the case the question to be asked is: Can or will the wonders of quantum mechanics be fully or even partially understood?

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Appendix

A Mathematica Program for computing the realigned matrix

Bipartite matrix (rho), that shall be realigned according to the dimension (dim) of one of the subsystems:

```
In[1]:= Realignbp[rho_, dim_] :=
 Table[
  Flatten[
   List[
    Flatten[
     Table[Flatten[Take[rho, {Mod[k * (Dimensions[rho][[1]] / dim) - (Dimensions[rho][[1]] / dim) + 1, Dimensions[rho][[1]], 1],
         Mod[k * (Dimensions[rho][[1]] / dim), Dimensions[rho][[1]], 1]}, {n}]],
      {n, If[Ceiling[k, dim] < dim, Ceiling[k, dim], If[dim == (Dimensions[rho][[1]] / dim), Ceiling[k, dim], (Dimensions[rho][[1]] / dim^2) * Ceiling[k, dim]]] -
        ((Dimensions[rho][[1]] / dim) - 1), If[Ceiling[k, dim] < dim, Ceiling[k, dim],
        If[dim == (Dimensions[rho][[1]] / dim), Ceiling[k, dim], (Dimensions[rho][[1]] / dim^2) * Ceiling[k, dim]]]}]]]], {k, 1, dim^2}]
```

Singular value of the realigned matrix:

```
In[2]:= SVRealign[rho_, dim_] := Plus @@ N[SingularValueList[Realignbp[rho, dim]]]
```

Examples:

```
In[3]:= rho2x2 := {{1, 2, 3, 4}, {5, 6, 7, 8}, {1, 3, 5, 9}, {2, 4, 6, 8}}

In[4]:= rho2x3 := {{1, 2, 3, 4, 5, 6}, {5, 6, 7, 8, 9, 10}, {1, 3, 5, 7, 8, 9}, {2, 4, 6, 8, 9, 10}, {7, 1, 2, 9, 3, 4}, {9, 8, 2, 3, 4, 6}}

In[5]:= rho2x2 // MatrixForm
```

Out[5]//MatrixForm=

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 1 & 3 & 5 & 9 \\ 2 & 4 & 6 & 8 \end{pmatrix}$$

```
In[6]:= Realignbp[rho2x2, 2] // MatrixForm
        1 / Tr[rho2x2] SVRealign[rho2x2, 2]
```

Out[6]//MatrixForm=

$$\begin{pmatrix} 1 & 5 & 2 & 6 \\ 1 & 2 & 3 & 4 \\ 3 & 7 & 4 & 8 \\ 5 & 6 & 9 & 8 \end{pmatrix}$$

```
Out[7]= 1.31539

In[8]:= rho2x3 // MatrixForm
```

Out[8]//MatrixForm=

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 5 & 6 & 7 & 8 & 9 & 10 \\ 1 & 3 & 5 & 7 & 8 & 9 \\ 2 & 4 & 6 & 8 & 9 & 10 \\ 7 & 1 & 2 & 9 & 3 & 4 \\ 9 & 8 & 2 & 3 & 4 & 6 \end{pmatrix}$$

```
        Realignbp[rho2x3, 2] // MatrixForm
        Realignbp[rho2x3, 3] // MatrixForm
```

Out[9]//MatrixForm=

$$\begin{pmatrix} 1 & 5 & 1 & 2 & 6 & 3 & 3 & 7 & 5 \\ 2 & 7 & 9 & 4 & 1 & 8 & 6 & 2 & 2 \\ 4 & 8 & 7 & 5 & 9 & 8 & 6 & 10 & 9 \\ 8 & 9 & 3 & 9 & 3 & 4 & 10 & 4 & 6 \end{pmatrix}$$

Out[10]//MatrixForm=

$$\begin{pmatrix} 1 & 5 & 2 & 6 \\ 1 & 2 & 3 & 4 \\ 7 & 9 & 1 & 8 \\ 3 & 7 & 4 & 8 \\ 5 & 6 & 7 & 8 \\ 2 & 2 & 9 & 3 \\ 5 & 9 & 6 & 10 \\ 8 & 9 & 9 & 10 \\ 3 & 4 & 4 & 6 \end{pmatrix}$$

B A simplex of bound entangled multipartite qubit states

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.

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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 $\Sigma_{i=1}^3 n_i^2=|\vec{n}|^2\leqslant 1$. For $|\vec{n}|^2<1$ the state is mixed (corresponding to Tr $\omega^2<1$) whereas for $|\vec{n}|^2=1$ the state is pure (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 $p_i\geqslant 0$, $\Sigma p_i=1$, otherwise it is entangled. As the property of separability does not change under local unitary transformation and classical communica-

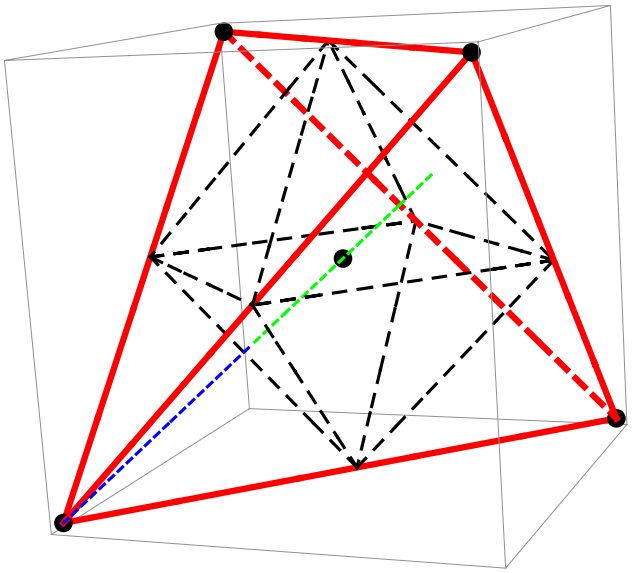

FIG. 1. (Color online) Here the geometry of the state space of even number of qubits is visualized. Each state is represent by a triple of three real numbers $\vec{c}$, Eq. (1). The four black dots at the vertices of the cube represent four orthogonal "vertex" states. In the case of two qubits these 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 $2\otimes 2$ and $2\otimes 3$ 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

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

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 $\rho \geqslant 0$ requires[1]

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

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

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

$$1 + \vec{c}\cdot\vec{n}^{(i)} \geqslant 0 \quad \text{with} \quad \vec{n}^{(i)} = \begin{pmatrix} -1 \\ +1 \\ +1 \end{pmatrix}, \begin{pmatrix} +1 \\ -1 \\ +1 \end{pmatrix}, \begin{pmatrix} +1 \\ +1 \\ -1 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix}. \tag{3}$$

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 $\mathrm{Tr}(\rho^2)$ 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 ($\mathrm{PT}_{\text{one qubit}}$) 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

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

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

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 $\mathrm{PT}_{\text{one qubit}}$.

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

$$\begin{aligned} E_{(2)}(\rho) &= E_{(12)}(\rho)+E_{(13)}(\rho)+\cdots+E_{(1n)}(\rho)+E_{(23)}(\rho)+\cdots \\ &\quad +E_{(2n)}(\rho)+\cdots+E_{(n-1,n)}(\rho), \\ E_{(3)}(\rho) &= E_{(123)}(\rho)+\cdots+E_{(n-2,n-1,n)}(\rho), \\ \cdots &= \cdots \\ E_{(n)}(\rho) &= E_{(12\cdots n)}(\rho). \end{aligned} \tag{9}$$

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

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

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 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 $|\mathrm{GHZ}\rangle$ states. Starting with one GHZ state, e.g.,

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

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 representation 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

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

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

$$
\begin{aligned}
&+\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_1i_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)
\end{aligned}
$$

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

$$
\begin{aligned}
\{i_1,i_2;i_1',i_2'\}=&\{0,1;0,0\},\{0,0;0,1\},\{0,1;1,0\},\{0,0;1,1\},\{1,1;0,0\},\{1,0;0,1\},\{1,1;0,0\},\{1,0;0,1\},\\
&\{0,0;1,0\},\{1,0;0,0\},\{0,0;1,1\},\{1,0;0,1\},\{0,1;1,0\},\{1,1;0,0\},\{0,1;1,1\},\{1,1;0,1\}. \quad (17)
\end{aligned}
$$

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

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

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

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

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

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

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 $1\geqslant c>\frac{1}{3}$ 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

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

and all parties get a copy state. Therefore, we reorder the state by a unitary transformation such that the first and second terms in the tensor product belongs to Alice and the third and fourth terms to Bob, and so on:

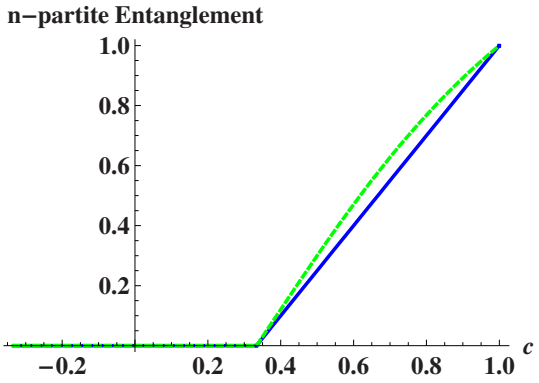

FIG. 2. (Color online) n-partite entanglement of the Werner states $n=2$ (here the y axis has to be multiplied by 2) or the generalized Smolin states $n>2$ before and after the application of the introduced protocol (upper dashed green curve). Note that the vertex states are mapped onto themselves by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

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

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

$$U_{\mathrm{XOR}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{25}$$

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

$$\vec{c} = \begin{pmatrix} c_x \\ c_y \\ c_z \end{pmatrix} \to \vec{c}_{\mathrm{dis}} = \begin{pmatrix} \frac{c_x^2 + c_y^2}{1+c_z^2} \\ \frac{2c_x c_y}{1+c_z^2} \\ \frac{2c_z}{1+c_z^2} \end{pmatrix}. \tag{26}$$

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 $-1/\sqrt{3}\leqslant c\leqslant 1/3$ 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

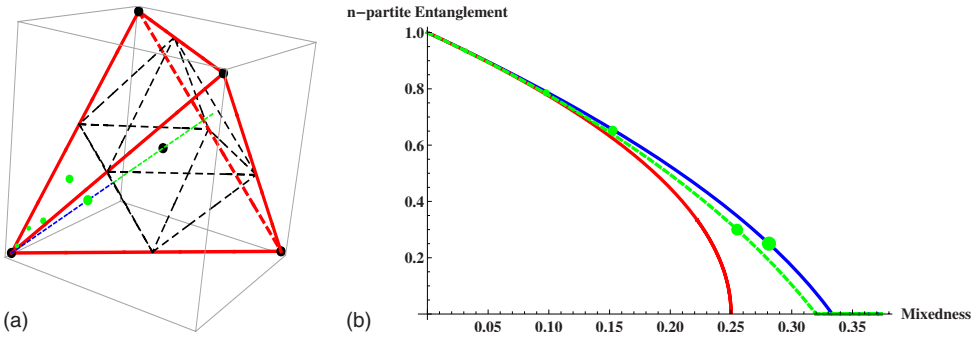

FIG. 3. (Color online) (a) Shows the final states after each step of the introduced protocol of an initial Werner or Smolin state $c=0.5$, where each (green) point represents the obtained state after one step of the protocol. (b) Shows the mixedness $[2^n/(2^n-1)][1-\mathrm{Tr}(\rho^2)]$, versus n-partite 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., $E(\rho_i')\leqslant E(\rho_i)\,\forall\,\Lambda$. And as the entanglement $E(\rho)$ is convex, i.e., $E(\rho_i')+E(\rho_j')\leqslant 2E(\rho_i')$, 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 furthermore, 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:

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

with

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

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 $\mathcal{M}(\rho)\geqslant 1$, 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.

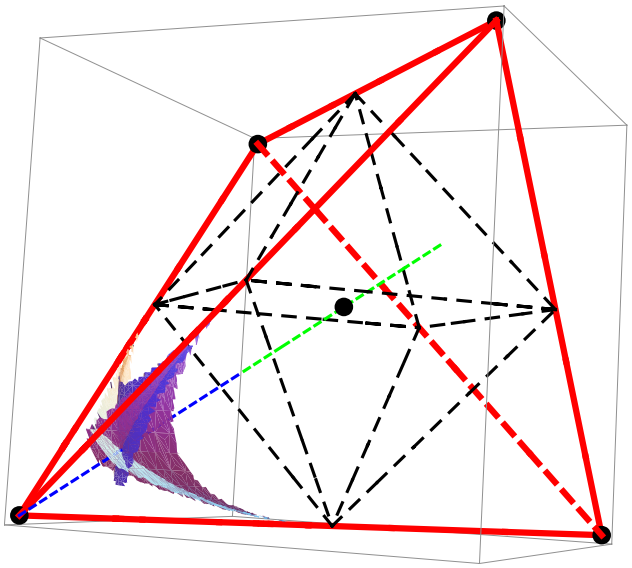

FIG. 4. (Color online) The three cylinders show the saturation of the Bell inequality. All states outside these cylinders violate the Bell inequality. The vertex states violate the Bell inequality maximally, i.e., by $2\sqrt{2}$.

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

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

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.

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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

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

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 $n=4,6,\ldots$.

Suppose Alice prepares her qubits in the following two states:

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

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:

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

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:

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

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

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

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

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

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:

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

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

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

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

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

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

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

$$\mathcal{O}^8 = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \otimes \sigma_x \otimes \sigma_y + \sigma_x \otimes \sigma_y \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_y \otimes \sigma_x \otimes \sigma_x\}. \quad \text{(B2)}$$

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

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

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

$$\mathcal{O}^{12} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \otimes \sigma_y \otimes \sigma_x - \sigma_y \otimes \sigma_x \otimes \sigma_y \otimes \sigma_x\}, \quad \text{(B3)}$$

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

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

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

$$\mathcal{O}^{16} = \frac{1}{4}\{\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_y + \sigma_x \otimes \sigma_y \otimes \sigma_x \otimes \sigma_y - \sigma_y \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y\}, \quad \text{(B4)}$$

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