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„Bound Entanglement Detection via Mutually Unbiased Bases and Symmetric Informationally Complete Positive Operator-Valued Measures in Qutrit Systems“

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Abstract

Detecting bound entanglement has lately become an important topic of research in the field of quantum information science. This special type of entanglement is undistillable meaning that it is not possible to obtain any pure entangled states from bound entangled states by means of LOCC (= local operations and classical communication). In this thesis, the detection of bound entanglement in several different families of states is considered which are located within a special state space, the so-called magic simplex. We focus here on bipartite qutrit systems.

The detection of entanglement is implemented by constructing entanglement witnesses using two different methods: Mutually Unbiased Bases (MUBs) and Symmetric Informationally Complete Positive Operator-Valued Measures (SIC-POVMs). MUBs are employed, e.g., in many protocols in QKD (quantum key distribution), because if a system is prepared in a state belonging to one of the MUBs, then all outcomes are equally likely when measured in another MUB, thus MUBs are maximally incompatible. SIC-POVMs, on the other hand, can be regarded as a particular case of a generalized quantum measurement on a Hilbert space. They have turned out to be very useful in current research areas like quantum state tomography as well as quantum cryptography.

The goal of this thesis is the (theoretical) detection of bound entanglement by utilizing a complete set of MUBs and SICs as two different but similar concepts to construct entanglement witnesses. Since both MUBs and SICs can be easily implemented in laboratory practice, the findings of this thesis concerning symmetry and bound entanglement pave the way to possible experimental applications and developments of quantum protocols based on MUBs or SICs.

Abstract (German)

Die Detektion von gebundener Verschränkung (engl. bound entanglement) hat sich unlängst zu einem wichtigen Forschungsfeld in der Quanteninformationstheorie entwickelt. Diese spezielle Art der Verschränkung ist nicht destillierbar, das heißt, es ist nicht möglich, reine verschränkte Zustände mithilfe von lokalen Operationen und klassischer Kommunikation aus gebunden verschränkten Zuständen zu gewinnen. In dieser Masterarbeit wird die Detektion von gebundener Verschränkung in mehreren Zustandsfamilien behandelt, welche sich in einem speziellen Zustandsraum befinden, dem sogenannten magischen Simplex. Wir betrachten hier ausschließlich bipartite Qutrit-Systeme, also eine Zweiteilchenverschränkung mit jeweils 3 Freiheitsgraden.

Der Nachweis von Verschränkung wird anhand von Verschränkungszeugen zweier unterschiedlicher Methoden erbracht: gegenseitig inkompatibler Basen (engl. Mutually Unbiased Bases, kurz MUBs genannt) und den symmetrischen informationsvollständigen positiven operatorwertigen Maßen (engl. Symmetric Informationally Complete Positive Operator-Valued Measures, kurz SIC-POVMs genannt). MUBs werden beispielsweise in vielen Protokollen in der Quantenschlüsselerzeugung benutzt, weil sie maximal inkompatibel sind: Wird ein System in einem Zustand einer solchen MUB präpariert und mithilfe einer anderen MUB anschließend gemessen, so treten alle möglichen Messergebnisse mit der gleichen Wahrscheinlichkeit ein. SIC-POVMs hingegen können als ein Spezialfall einer generalisierten Quantenmessung auf einen Hilbertraum angesehen werden. Sie haben sich zuletzt in aktuellen Forschungsfeldern wie der Quantentomographie und auch der Quantenkryptographie als äußerst nützlich erwiesen.

Das Ziel dieser Masterarbeit ist die (theoretische) Erfassung von gebundener Verschränkung mithilfe vollständiger Mengen von MUBs und SICs als zwei unterschiedliche, aber ähnliche Konzepte zur Konstruktion von Verschränkungszeugen. Sowohl MUBs als auch SICs können im Labor, im Vergleich zu anderen Methoden, auf einfache Weise implementiert werden. Darum können die Ergebnisse der hier erbrachten Studie bezüglich Symmetrie und gebundener Verschränkung für mögliche experimentelle Anwendungen genutzt werden, aber auch zur Entwicklung von Quantenprotokollen basierend auf MUBs oder SICs.

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1 Introduction

Studying and utilizing quantum entanglement is currently one of the most active fields of research in physics. In the last two decades tremendous progress has been made in quantum information theory to understand the different kinds of entanglement in order to utilize them in quantum communication protocols as well as quantum computation. As one of the most important non-classical and counter-intuitive phenomena in quantum physics, the steadily increasing interest in entanglement will make it the main resource in many future technologies. However, detecting entanglement is in general an NP-hard problem which constitutes one of the most complex problems in mathematics and computational science, and is therefore anything but easy to resolve.

Entanglement is called the property of a quantum system whose state cannot be written as a product of states of its local (spatially separated) subsystems such as photons or electrons. This means, for a bipartite system the two particles cannot be described independently of each other. Due to their correlations they can only be characterized as a whole which consequently means that the total system contains more information than the individual subsystems.

First, the implications of entanglement were rejected by Einstein, Podolsky and Rosen in 1935, who tried to explain this unknown and inexplicable property by a possible incompleteness of the quantum mechanical description of physical processes [1]. It was John Bell in 1964 who clearly showed that the phenomenon of entanglement indeed leads to deviations of the predictions of quantum theory and the predictions of classical physics which are measurable in experiment. Thus, Bell finally proved the doubts of Einstein, Podolsky and Rosen about the completeness of quantum mechanics wrong [2]. It took another thirty years before Asher Peres showed a necessary condition for separable states: The partial transposition of such states only has non-negative eigenvalues which is a stronger criterion than Bell's inequality [3]. Shortly thereafter the Horodecki family extended this criterion of separability: For 2×2 and 2×3 quantum systems the positivity of the partial transposition (PPT) of a state is not only necessary but also sufficient for its separability. However, in systems of higher dimension, i.e. $d_{tot} > 6$, this generally does not hold [4]. Hence, there can exist some mixed states which fulfill this partial transposition criterion although they are entangled. Thus we have undistillable entanglement because the Horodecki family further proved that if a mixed state can be distilled to the singlet form, it must violate the partial transposition criterion [5]. Consequently there are two qualitatively different types of entanglement: the already known "free" or distillable entanglement and the so-called "bound" or undistillable entanglement. As far as we know, this kind of entangled states, also known as PPT-entangled states, cannot be used alone in quantum communication, such as quantum cryptography.

Detection of bound entanglement is the main topic of this thesis. The meaning of this undistillable entanglement in nature is still not understood because generating such states needs pure entanglement but, once created, it is not possible to retrieve any pure entanglement from them. However, one has lately managed to produce bound entanglement of two photon qutrits and thereby showed the first successful experimental detection of these heavily mixed entangled states [6]. While the study presented here will utilize the partial transposition criterion as a necessary condition bound entangled states have to meet, it should be noted that there might also be bound entangled states that are negative under partial transposition (NPT) - see for

example Ref. [7] and the references therein for more information about this. But in general, the existence of NPT bound entanglement is still an open mathematical (and physical) issue. Due to the fact that distillability of entanglement plays an important role in many tasks in quantum information theory, like quantum cryptography or teleportation, one could think that there is no use for bound entangled states. Nevertheless, the last two decades have pointed out that there are quite a few applications for such states in quantum information science, e.g. for drawing a cryptographically private key [8], or as additional source in entanglement activation [9]. More recently, it has been found out that bound entangled states can be very useful in quantum metrology [10, 11].

In this thesis, the detection of bound entanglement by employing entanglement witnesses is addressed. Those witnesses are constructed via two different but equivalent methods: Mutually Unbiased Bases (MUBs) and Symmetric Informationally Complete Positive Operator-Valued Measures (SIC-POVMs). MUBs are very handy, in particular for experimenters, in order to explore Bohr's complementarity since measuring a state belonging to one of the MUBs will provide maximal uncertainty about another state if this one is prepared in another MUB from the same set [12]. SIC-POVMs can also be very useful in quantum state tomography and quantum cryptography. While an informationally complete POVM determines completely the quantum state on which the measurements are carried out, a SIC-POVM is characterized by the condition that all pairwise inner products between the POVM elements, i.e. the measurement operators, are equal [13]. So MUBs and SICs alike are maximally incompatible. For both of them there are certain criteria for the upper bound on the set of separable states based on which MUB-entanglement witnesses and SIC-entanglement witnesses respectively can be created. The aim of this thesis is finding bound entanglement by applying MUB- and SIC-witnesses to various bipartite qutrit families of states which are characterized by different parameterizations. All of those states are embedded within the so-called magic simplex, a highly symmetric subspace of the Hilbert space.

In the following chapter a short repetition of the essential mathematical (and physical) background is provided. This is necessary to understand the further sections of the thesis. The third chapter covers the difference between separability and entanglement in bipartite systems in detail. In this context the positive partial transpose criterion (PPT-criterion) is precisely explained so that the idea of bound entanglement can be introduced. Furthermore, we will treat the notion of entanglement witnesses and discuss their general properties. Chapter 4 provides a definition of the mutually unbiased bases (MUBs) and describes their relevant properties while chapter 5 deals in a similar way with the symmetric informationally complete positive operator-valued measures (SIC-POVMs). For simplicity, only one way of constructing MUBs and SIC-POVMs, respectively, is addressed and used throughout this study. Then the focus is set on the generation of entanglement witnesses - first via a complete set of MUBs and then via a full set of SICs. In addition, the last subsection of chapter 5 considers the fact that both MUBs and SICs are subsets of a so-called quantum 2-design which explains their equivalence (for a total set of both methods). In chapter 6, the magic simplex is first defined and its most relevant properties are explained. Afterwards we analyze the ability of MUB- and SIC- witnesses detecting bound entanglement when applied to different families of states with different numbers of parameters, located

within the magic simplex. In this thesis only bipartite systems, to be more precise, bipartite qutrits are considered. The outcomes of the (optimized) entanglement witnesses are compared among the MUB- and SIC-witnesses respectively and then the two methods. For some classes of states, that is for some slices through the magic simplex, the quality, i.e. the efficiency in detecting (or non-detecting) bound entanglement, of a few witnesses is visualized in order to give a graphic intuition.

A brief summary of the findings and an outlook are given in the last chapter, as well as a large overall table with all the main results presented in this thesis.

2 Foundations

First of all, we will review some mathematical basics necessary to comprehend the subjects described in the subsequent chapters.

2.1 Density Matrix Formalism

Let us consider a d -dimensional Hilbert space $\mathcal{H} = \mathbb{C}^d$ with the Hilbert-Schmidt inner scalar product defined by

$$\langle A|B \rangle = \text{Tr}(A^\dagger \cdot B). \quad (2.1)$$

Such a linear vector space of operators is called the Hilbert-Schmidt space which is a Hilbert space as well. Its elements, the Hilbert-Schmidt operators, have to satisfy the standard Hilbert-Schmidt norm

$$\|A\| = \sqrt{\langle A|A \rangle}. \quad (2.2)$$

In quantum information (and in general quantum mechanics) one uses the density matrix formalism in order to represent pure and mixed states. The density matrix ρ as a Hilbert-Schmidt operator $\rho \in \mathcal{H}$ has to fulfill the following properties:

1. $\text{Tr}(\rho) = 1$ (normalization)
2. $\rho \geq 0$ (positivity) $\Rightarrow \rho = \rho^\dagger$ (hermiticity)

While a pure state where we have complete information about the state can be described as the simple outer product of the vector state $|\psi\rangle \in \mathcal{H}$:

$$\rho = |\psi\rangle\langle\psi| \quad (2.3)$$

and thus $\rho^2 = \rho$ and $\text{Tr}(\rho^2) = 1$, a mixed state contains only partial knowledge about the state and is therefore characterized by a convex combination of pure states $\{|\psi_i\rangle\}$:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad (2.4)$$

with the probabilities $p_i \geq 0$ and $\sum_i p_i = 1$. Obviously, we have in this case $\rho^2 \neq \rho$ and thus $\text{Tr}(\rho^2) < 1$.

In this work we will represent the density matrix by the Bloch vector decomposition of qudits (Bloch vector expansion of the density matrix [14]):

$$\rho = \frac{1}{d} \mathbb{1} + \vec{b} \cdot \vec{\Gamma}, \quad (2.5)$$

where the components of the Bloch vector $b_i = \langle \Gamma_i \rangle = \text{Tr}(\rho \cdot \Gamma_i)$ are in general complex and $\vec{b} \cdot \vec{\Gamma}$ denotes a linear combination of the matrices $\{A_i\}$. All of those matrices $\{A_i\}$ of dimension $d \times d$ are supposed to be traceless, i.e. $\text{Tr}(A_i) = 0$, and orthogonal, i.e. $\text{Tr}(A_i^\dagger A_j) = N \delta_{ij}$ with $N \in \mathbb{R}$. One representation of $\{A_i\}$ are the $d^2 - 1$ hermitian Gell-Mann matrices with $\vec{b} \in \mathbb{R}^{d^2-1}$. Another one are the d^2 unitary but not hermitian Weyl operators that are used in this thesis, see (2.14), with $\vec{b} \in \mathbb{C}^{d^2}$. Exploiting $\text{Tr}(\rho^2) \leq 1$, it follows that $|\vec{b}| \leq \frac{\sqrt{d-1}}{d}$.

The Bloch vector expansion of a density matrix $\rho \in \mathcal{H} = \mathbb{C}^d$ bears the advantage that it can be used likewise for pure and mixed states. However, in higher dimensions, i.e. $d > 2$, any state ρ can be represented by $\vec{b}$ but not every $\vec{b}$ corresponds to a state, that is a density matrix. The problem is that the conditions $\text{Tr}(\rho) = 1$ and $\text{Tr}(\rho^2) \leq 1$ do not generally imply the positivity of ρ . Therefore, in higher dimensions there is also a Bloch (hyper)sphere as we have for qubits but this sphere contains points ("holes") where ρ shows negative eigenvalues which cannot be considered as a physical state.

So far we have only discussed single systems but in this thesis we deal with bipartite systems, i.e. $\rho = \rho_A \otimes \rho_B$ where $\rho_A \in \mathcal{H}_A$ and $\rho_B \in \mathcal{H}_B$, thus we have $\rho \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. In such a bipartite qudit system with $\mathcal{H} = \mathbb{C}^d$ the Bloch vector decomposition of ρ looks like the following

$$\begin{aligned} \rho = \rho_A \otimes \rho_B &= \left(\frac{1}{d}\mathbb{1} + \vec{a} \cdot \vec{\Gamma}\right) \otimes \left(\frac{1}{d}\mathbb{1} + \vec{b} \cdot \vec{\Gamma}\right) = \\ &= \frac{1}{d^2}(\mathbb{1} \otimes \mathbb{1}) + \frac{1}{d} \left(\sum_i a_i \Gamma_i \otimes \mathbb{1} + \sum_i b_i \mathbb{1} \otimes \Gamma_i \right) + \sum_{ij} a_i b_j \Gamma_i \otimes \Gamma_j, \end{aligned} \quad (2.6)$$

where $a_i, b_i \in \mathbb{C}$ and $\{\Gamma_i\}$ indicates a basis in the subspace $\mathcal{H}_A$ (analogously in $\mathcal{H}_B$) like the Gell-Mann matrices or Weyl operators. This formalism for denoting the state of a bipartite system is essential in quantum information theory and will be used in the following chapters to describe the family of isotropic states, the magic simplex as well as all other families of states in the magic simplex presented in this study.

2.2 Weyl Basis

There are two common representations in order to find appropriate matrices for $\vec{\Gamma}$ given in eq.(2.5), at least for bipartite qutrits ($d = 3$): the Gell-Mann matrices and the Weyl matrices. Both of them can be thought of as generalizations of the Pauli matrices in $d = 2$, i.e. for qubits. And both of them have advantages and disadvantages and it depends on the context which one is the better choice. This thesis works exclusively with the Weyl operator basis which consists of d^2 operators defined as follows [14]:

$$W_{kl} = \sum_{j=0}^{d-1} \omega^{jk} |j\rangle \langle (j+l) \bmod d|, \quad k, l = 0, 1, \dots, d-1 \quad (2.7)$$

$$\text{Tr}(W_{mn}^\dagger W_{kl}) = d \delta_{mk} \delta_{nl}, \quad (2.8)$$

where $\omega = e^{\frac{2\pi i}{d}}$ marks the d -th root of unity with the relation $\sum_{j=0}^{d-1} \omega^j = 0$ and $\{|j\rangle\}_{j=0}^{d-1}$ is the standard basis of $\mathbb{C}^d$.

As eq.(2.8) clearly shows, the Weyl operators are unitary and establish an orthonormal basis of the Hilbert–Schmidt space. However, they are not hermitian. So, unlike Gell-Mann matrices (which are not unitary instead), they do not directly refer to observables. Furthermore the Weyl operators obey the Weyl relations [15]:

$$W_{m,l} W_{k,n} = \omega^{kl} W_{m+k, l+n} \quad (2.9)$$

$$W_{k,l}^\dagger = W_{k,l}^{-1} = \omega^{kl} W_{-k,-l} \quad (2.10)$$

$$W_{0,0} = \mathbb{1}. \quad (2.11)$$

The Weyl operators are very handy in quantum information theory because they can be used to form a basis of d^2 maximally entangled qudit states: If we apply W_{kl} to any maximally entangled pure state written, e.g., in the form

$$|\Omega_{00}\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |j\rangle \otimes |j\rangle, \quad (2.12)$$

which represents a generalized Bell state, we can find further maximally entangled states. Indeed, using eq.(2.12) as the seed state we can receive all of the remaining d^2 Bell states $|\Omega_{kl}\rangle$ in the respective dimension via

$$|\Omega_{kl}\rangle = (W_{kl} \otimes \mathbb{1})|\Omega_{00}\rangle. \quad (2.13)$$

Thus, we receive a complete orthonormal basis (ONB) of maximally entangled states just by implementing this simple operation. Later, when introducing the magic simplex and trying to detect bound entanglement the Weyl operators will be of great importance.

Since this thesis addresses bipartite qutrits only, let us explicitly depict the form of the Weyl matrices for $d = 3$:

$$\begin{aligned} W_{00} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & W_{01} &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, & W_{02} &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, & (2.14) \\ W_{10} &= \begin{pmatrix} \omega & 0 & 0 \\ 0 & \omega^* & 0 \\ 0 & 0 & 1 \end{pmatrix}, & W_{11} &= \begin{pmatrix} 0 & \omega & 0 \\ 0 & 0 & \omega^* \\ 1 & 0 & 0 \end{pmatrix}, & W_{12} &= \begin{pmatrix} 0 & 0 & \omega \\ \omega^* & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \\ W_{20} &= \begin{pmatrix} \omega^* & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & 1 \end{pmatrix}, & W_{21} &= \begin{pmatrix} 0 & \omega^* & 0 \\ 0 & 0 & \omega \\ 1 & 0 & 0 \end{pmatrix}, & W_{22} &= \begin{pmatrix} 0 & 0 & \omega^* \\ \omega & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \end{aligned}$$

2.3 LOCC

Since bound entanglement can be defined as entanglement that cannot be distilled by local operations and classical communication (LOCC), i.e. no pure entanglement can be obtained from bound entangled states by means of LOCC, we will take a short look at this type of operations.

We consider a bipartite qubit system with the observers Alice A and Bob B who share one of two possible pure maximally entangled states (Bell states):

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B) \quad (2.15)$$

$$|\phi^-\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |0\rangle_B - |1\rangle_A \otimes |1\rangle_B), \quad (2.16)$$

where $|i\rangle_A \in \mathcal{H}_A$ and $|i\rangle_B \in \mathcal{H}_B$ with $i = \{0, 1\}$ and the bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{H}$. Neither Alice nor Bob knows which state their joint system is in so they use LOCC operations to find it out: One of the observers, e.g. Alice, measures her qubit, i.e. she performs a local operation on her part of the common system which evolves independently from Bob's subsystem, and then sends her result via classical communication to Bob. He will now measure his qubit thus implementing a local operation on his subsystem and, based on the information he has received from Alice, they can determine the Bell state they share.

Naturally, this idea can also be applied to far more complex protocols: Having access to different subsystems several parties can use classical communication to exchange information about their locally performed measurements and their outcomes. Then they can conduct further local operations conditioned on the communicated information they have received [16].

LOCC operations are very useful due to their local implementation. The concept of entanglement is related to the non-local properties of a physical state, therefore local quantum operations (with classical correlations between the subsystems) cannot affect the intrinsic nature of entanglement [17]. Thus, by using LOCC a separable state (product state) will always remain separable but entangled states and in general quantum correlations cannot be created by means of LOCC operations. That is also the reason why a common property of an entanglement measure is that the amount of entanglement in a quantum state cannot be increased by LOCC operations.

So one can use LOCC to transform separable states into other separable states and likewise entangled states into other entangled states. Mathematically, such a local symmetry is stated as follows:

$$\rho'_{sep} = (U_1 \otimes U_2)\rho_{sep}(U_1 \otimes U_2)^\dagger = \rho_{sep} \quad (2.17)$$

$$\rho'_{ent} = (U_1 \otimes U_2)\rho_{ent}(U_1 \otimes U_2)^\dagger = \rho_{ent}, \quad (2.18)$$

where $\rho_{sep} \in \mathcal{H}$ denotes a separable and $\rho_{ent} \in \mathcal{H}$ an entangled bipartite quantum state. Both are left invariant under any local unitary transformation of the form $U = U_1 \otimes U_2$.

3 Entanglement in Bipartite Systems

This chapter will only cover the mathematical and physical explanation of bipartite entanglement since the study presented here just concerns bipartite qutrits. Naturally, bipartite entanglement is much less complex than multipartite entanglement because here we have a true distinction between separable and entangled states and nothing in between like the partial separability. But due to the fact that detecting bound entanglement by means of MUBs or even SIC-POVMs is still poorly understood it is better to stick to the simplest case where this type of entanglement can emerge: bipartite qutrits. Nevertheless, the results presented here could serve as a basis for a study on the detection of multipartite bound entanglement.

3.1 Separability vs. Entanglement

Using the density matrix formalism, introduced in chapter 2.1, we will first explain the difference between separable and entangled states.

Let us assume a bipartite quantum system described by the Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ where $\mathcal{H}_A$ marks the Hilbert space of Alice's subsystem with dimension d_A and, analogously, $\mathcal{H}_B$ the Hilbert space of Bob's subsystem with dimension d_B . The Hilbert space $\mathcal{H}$ of the composite system thus has dimension $d = d_A d_B$. Now we can define:

A pure bipartite quantum state $|\psi\rangle \in \mathcal{H}$ is called separable or product state if it can be written as

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle, \quad (3.1)$$

where $|\psi_A\rangle \in \mathcal{H}_A$ and $|\psi_B\rangle \in \mathcal{H}_B$. Physically, one can consider product states as uncorrelated states meaning that Alice's state $|\psi_A\rangle$ acts independently from Bob's state $|\psi_B\rangle$.

If $|\psi\rangle$ cannot be put in the form of the above eq.(3.1) the state is called entangled. Examples of such pure states are the Bell states, the four maximally entangled states of two qubits. Two of them are depicted in the equations (2.15) and (2.16).

However, generally one has to deal with mixed states since one does not know the exact state of a quantum system. In such a case, there are only some probabilities p_i which relate to the different possible (pure) states $|\psi_i\rangle \in \mathcal{H}$. Then one uses a density matrix $\rho \in \mathcal{H}$, formulated in eq.(2.4), in order to describe this situation as a (convex) combination of pure states. Consequently, for defining separability and entanglement for mixed states one uses the same idea as for pure states: A state is called separable if and only if it can be produced locally, if not it is entangled.

A mixed bipartite quantum state ρ is called separable if it can be written as

$$\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B, \quad (3.2)$$

where $\{p_i\}$ is the probability distribution (with $p_i \geq 0$ and $\sum_i p_i = 1$) and $\rho_i^A \otimes \rho_i^B$ denotes the product states of Alice's subsystem, $\rho_i^A \in \mathcal{H}_A$, and Bob's subsystem, $\rho_i^B \in \mathcal{H}_B$.

If ρ cannot be put in such a factorization of its distinct subsystem's states, as it is given in the form of eq.(3.2), the state is called entangled.

Since any state can be represented by a density matrix, i.e. a positive semidefinite matrix of trace one, all states form a convex set. As one can see by the definition of separability, all separable states compose a convex set as well. Hence, the combination of two separable states

results in another separable state and the set of separable states is the convex subset of the (convex) set of all states. So its extremal points, the pure separable states, are located on the border of the the total set [18]. From this it follows that the closed set of separable states is surrounded by the set of entangled states since in bipartite systems a state is either entangled or separable.

Since separable states are classically correlated, LOCC (defined in section 2.3) can be used to produce them while entanglement cannot be obtained by any classical processes. Quantum correlations are required for this.

As can be seen by the equations above we only have clear definitions for separability but none for entangled states. Indeed, so far, there is no definite formulation of a general, i.e. mixed, entangled state known, therefore it is not possible to determine whether a given state is entangled or separable. We can only set up criteria that are based on separability which means that they are fulfilled for all separable states. If there is now a state that violates such a separability criterion we can conclude that this state is truly entangled but if the criterion is satisfied we cannot tell anything about it.

However, there is one family of states where we can clearly differentiate between separable and entangled states: the isotropic states. They are invariant under any transformation $U_A \otimes U_B^*$ where A and B represent the observables acting in the subsystems $\mathcal{H}_A$ and $\mathcal{H}_B$ of the bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$. Generally, isotropic density matrices are convex mixtures of a maximally entangled state and the maximally mixed state [19]:

$$\rho_\alpha = \alpha |\phi_+^d\rangle\langle\phi_+^d| + (1 - \alpha) \frac{\mathbb{1}_d \otimes \mathbb{1}_d}{d^2}, \quad (3.3)$$

where $\alpha \in \mathbb{R}$ has to fulfill the condition $-\frac{1}{d^2-1} \leq \alpha \leq 1$ due to the positivity of the state and $|\phi_+^d\rangle$ is a maximally entangled state defined by

$$|\phi_+^d\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle_A \otimes |i\rangle_B, \quad (3.4)$$

where $\{|i\rangle\}_{i=0}^{d-1}$ denotes an orthonormal basis in $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and d is the subsystem's dimension.

Since all entangled isotropic states violate the so-called reduction criterion, another separability criterion concerning positive but not completely positive maps (see Ref. [20] for a closer look) we can set up the following properties for isotropic states:

$$\begin{aligned} -\frac{1}{d^2-1} \leq \alpha \leq \frac{1}{d+1} &\Rightarrow \rho_\alpha \text{ separable}, \\ \frac{1}{d+1} < \alpha \leq 1 &\Rightarrow \rho_\alpha \text{ entangled}. \end{aligned} \quad (3.5)$$

That is the reason why isotropic states are characterized as a one-parameter family of states. Still, such classes of states where we can certainly say which states are separable and which are entangled by easy conditions like this here are very rare exceptions.

The fact that there is still no general necessary criterion for entanglement is one of the greatest

problems in quantum information theory, the so-called separability problem. By now, many different separability criteria have been developed but we will only discuss those that are necessary for this thesis. In the next chapter we will treat the most known one, the Peres-Horodecki criterion or PPT criterion, and then another one that will be essential for defining the MUB- and the SIC-entanglement witnesses. This special separability criterion will therefore be explained in section 3.4.

3.2 The PPT criterion

In order to understand the PPT criterion one has to deal with positive and completely positive maps.

Let us consider a bipartite Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ where $\mathcal{A}(\mathcal{H}_i)$ with $i = \{1, 2\}$ denotes the set of linear operators acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. A map $\Lambda : \mathcal{A}(\mathcal{H}_1) \rightarrow \mathcal{A}(\mathcal{H}_2)$ is called positive if it maps positive operators onto positive operators, satisfying

$$A \geq 0 \Rightarrow \Lambda(A) \geq 0, \quad (3.6)$$

where $A \in \mathcal{A}(\mathcal{H}_1)$. Now, a positive map is called completely positive, if it remains positive under the extension $\Lambda \otimes \mathbb{1}_A(A)$ for any positive A :

$$A \geq 0 \Rightarrow \Lambda \otimes \mathbb{1}_A(A) \geq 0, \quad (3.7)$$

where $\mathbb{1}_A(A)$ marks the identity matrix on $\mathcal{A}(\mathcal{H}_A)$ for an arbitrary Hilbert space $\mathcal{H}_A$.

It has been shown in Ref. [4] that any positive map of a separable state ρ_{sep} is also completely positive:

$$\Lambda(\rho_{sep}) \geq 0 \Rightarrow (\Lambda \otimes \mathbb{1})(\rho_{sep}) = (\Lambda \otimes \mathbb{1})\left(\sum_i p_i \rho_i^A \otimes \rho_i^B\right) = \sum_i p_i \Lambda(\rho_i^A) \otimes \rho_i^B \geq 0. \quad (3.8)$$

This explains why positive maps can serve as a separability criterion: If and only if eq.(3.8) is fulfilled for all positive maps the general state ρ is separable, however, if there exists a positive map Λ such that $(\Lambda \otimes \mathbb{1})(\rho) \not\geq 0$, this state is considered as inseparable or entangled. But as a separability criterion, eq.(3.8) cannot be employed in order to determine whether a given state is entangled or not, thus it is also possible that there exist entangled states ρ_{ent} satisfying $(\Lambda \otimes \mathbb{1})(\rho_{ent}) \geq 0$.

One of the most important positive but not completely positive maps in quantum information theory is the partial transposition which was first introduced by Peres in Ref. [3].

Generally, any state ρ of a composite system can be extended into a chosen product basis:

$$\rho = \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d-1} \rho_{ij,kl} |i\rangle\langle j| \otimes |k\rangle\langle l| = \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d-1} \rho_{ij,kl} |ik\rangle\langle jl|. \quad (3.9)$$

Here we have used a simpler notation: $|ab\rangle = |a\rangle \otimes |b\rangle$ and analogously $\langle ab| = \langle a| \otimes \langle b|$.

Now one can use this decomposition in order to define the partial transpose of the bipartite state ρ , that is the transposition T with respect to one subsystem while the other one is left

unchanged. So we have two possible partial transpose operations, one for Alice A that looks like

$$\rho^{T_A} = \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d-1} \rho_{ji,kl} |ik\rangle \langle jl| = \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d-1} \rho_{ij,kl} |jk\rangle \langle il|, \quad (3.10)$$

and one for Bob's subsystem B:

$$\rho^{T_B} = \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d-1} \rho_{ij,lk} |ik\rangle \langle jl| = \sum_{i,j=0}^{d-1} \sum_{k,l=0}^{d-1} \rho_{ij,kl} |il\rangle \langle jk|. \quad (3.11)$$

Naturally, one has $(\rho^{T_A})^{T_B} = (\rho^{T_B})^{T_A} = \rho^T$. It shall be noticed that the partial transpose does depend on the basis in which it is performed but its spectrum does not which also holds for the usual (total) transpose.

A state is called PPT, i.e. it has positive partial transpose, if none of the eigenvalues of its partial transpose is negative, that is the state remains positive semidefinite under partial transposition:

$$\rho^{T_A} \geq 0 \Leftrightarrow \rho^{T_B} \geq 0. \quad (3.12)$$

Conversely, the state is called NPT if it is non-positive under partial transposition, i.e. not PPT.

Using these definitions we can now formulate the PPT criterion, also known as the Peres-Horodecki criterion [3]: If a bipartite state ρ is separable, then ρ is PPT.

This means that NPT states are certainly entangled. Thus, by simply calculating the partial transpose of a bipartite state with respect to one subsystem, and finding at least one negative eigenvalue means that this state is entangled. So this separability criterion serves as an easy but also a very efficient tool for the detection of entanglement in bipartite systems. However, it has turned out that the PPT criterion is necessary and sufficient in 2×2 or 2×3 systems only, i.e. if the dimension of the composite system is $d = d_A d_B \leq 6$. In higher dimensions, $\rho^{T_A} \geq 0$ is just a necessary condition for separability but no longer a sufficient one. Hence, in systems with $d_A d_B > 6$ a PPT state can be separable or entangled. This explains the existence of a special sort of entanglement, the so-called bound entanglement, that stays positive semidefinite under partial transposition which will be discussed in more detail in the following section.

The reason why the PPT criterion is necessary and sufficient just in systems of two qubits or of one qubit and one qutrit is that no positive map other than transposition is needed to detect all of the entangled states. In such low dimensions all positive maps Λ are decomposable which can be written in the form $\Lambda = \Lambda_A^{CP} + \Lambda_B^{CPT}$ where Λ_i^{CP} with $i = \{A, B\}$ represents a completely positive map. In Ref. [4] it is shown that a bipartite state that is not positive under any of these maps, i.e. every possible entangled state, must be NPT. So in bipartite systems having dimensions 2×2 or 2×3 , $\rho^{T_A} \geq 0$ definitely implies separability only.

3.3 Bound Entanglement

In real-world quantum communication experiments one always has to deal with mixed states and not pure states because noise is unavoidable which may cause decoherence effects. Thus,

Alice and Bob cannot share pure maximally entangled states as it is required by many procedures and protocols in quantum information theory. One needs to purify a given bipartite entangled mixed state into a maximally entangled one by LOCC which is called distillation of entanglement:

If many copies of an entangled mixed state ρ can be purified or distilled into fewer maximally entangled states via LOCC, then this state is called distillable:

$$\rho^{\otimes m} \xrightarrow{LOCC} |\phi_+^d\rangle, \quad (3.13)$$

where $\rho^{\otimes m}$ represents m copies of the state ρ and $|\phi_+^d\rangle$ denotes a maximally entangled state (see eq.(3.4)). However, there exist states that are entangled but not distillable. This special form of entanglement is known as undistillable or bound entanglement.

As far as we know, all free or distillable entangled states are NPT states. Therefore, bound entangled states are positive under partial transposition although they are not separable. Since we already know that the PPT criterion works as a necessary and sufficient separability criterion in 2×2 or 2×3 systems, bound entangled states do not exist there. Consequently, bipartite qubit systems cannot produce any bound entanglement but higher dimensional systems like bipartite qutrits can. In multipartite qubit systems, i.e. more than two particles, however, bound entangled states can emerge but this multipartite bound entanglement differs substantially from the bipartite one and will not be considered here (see e.g. Ref. [21]).

Hence, the PPT criterion serves as a necessary and sufficient criterion for the non-distillability of a state. Trying to find bipartite bound entangled qutrit states thus means satisfying three conditions: They have to be positive, PPT and entangled. Detecting these so-called PPT entangled states will be the main goal of this thesis. There may also exist NPT bound entangled states because the violation of the PPT criterion does not automatically imply the distillability of a state. But NPT bound entanglement is a still controversially discussed problem and will not be covered here (for more information about that topic see Ref. [7, 22, 23]).

To this day, there are no methods known how to (generally) construct bound entangled states and even their purpose in nature is still mysterious. In quantum communication processes this undistillable entanglement proves to be an obstacle: First, one needs entanglement in order to create bound entangled states and afterwards it is impossible to retrieve any maximal entanglement via LOCC from them. So, while the opposite way of eq.(3.13) with many copies of the maximally entangled state $|\phi_+^d\rangle$ holds, eq.(3.13) itself does not. In other words, bound entangled states cannot be distilled to a maximally entangled one which also explains their name: contrary to free entanglement, bound entanglement is not unlockable.

On the other hand, due to its strange behaviour and our still little knowledge about it, bound entanglement is of great interest in quantum information science. Moreover, bound entangled states can be very practical since, as one of several applications, their entanglement can be, in a sense, activated if they are used together with distillable entangled states [9]. They can also be used for secure quantum key distribution, e.g. establishing an arbitrarily secure key from bound entangled states [24]. One can see that characterizing and detecting bound entanglement is a fascinating but also challenging and important task in quantum informational studies.

When investigating our chosen families of bipartite qutrit states located within the magic simplex in search of bound entanglement, we have to find, first, the region of positivity, and second, the region of PPT. Due to the fact that states meeting the PPT criterion can be

separable or bound entangled, it is clear that the domain of bound entanglement lies closer to the one of separable states than the range of free entanglement - in fact, it encloses the region of separability. Therefore, bound entanglement is a weaker type of entanglement, that is of lower purity than free entanglement.

Accordingly, in order to ascertain whether PPT states are indeed entangled, we need further tools. This brings us to the concept of entanglement witnesses.

3.4 Entanglement Witnesses

In the context of entanglement detection we need to discuss a criterion for the entanglement of a state which can also be viewed as a different type of separability criteria: the entanglement witnesses. As the name already implies, these operators are supposed to detect entanglement, that is, ideally, to separate the set of separable states from the entangled ones. In general, an entanglement witness $\mathcal{W}$ is defined by a hermitian operator $\mathcal{W} = \mathcal{W}^\dagger$, i.e. an observable, which satisfies the following inequalities:

$$Tr(\mathcal{W}\rho_{ent}) < 0 \quad (3.14)$$

$$Tr(\mathcal{W}\rho_{sep}) \geq 0, \quad \forall \rho_{sep} \in S, \quad (3.15)$$

where S marks the set of all separable states ρ_{sep} and ρ_{ent} indicates an entangled state. As a consequence of the Hahn-Banach-theorem [4] there exists an entanglement witness for each entangled state detecting it. While eq.(3.14) only holds for some entangled states, or to be more accurate, for at least one entangled state, eq.(3.15) has to be valid for all separable states. However, eq.(3.15) is in general very difficult to prove because it is an NP-hard problem, i.e. a problem which is at least as hard as the hardest problems in NP (= non-deterministic polynomial-time). On the other hand, given the proof was successful for a particular witness, we know by $Tr(\mathcal{W}\rho) < 0$ that this (generally mixed) state ρ is indeed entangled and then we can say that the state ρ is detected by our entanglement witness $\mathcal{W}$.

Now, an entanglement witness is called "optimal", represented by $\mathcal{W}_{opt}$, if there exists at least one separable state $\tilde{\rho}_{sep} \in S$ such that

$$Tr(\mathcal{W}\tilde{\rho}_{sep}) = 0. \quad (3.16)$$

This implies that there exists no finer entanglement witness than $\mathcal{W}_{opt}$ where 'finer witness' $\mathcal{W}_{finer}$ means that it can detect all entangled states of a certain witness $\mathcal{W}$ and, in addition, some more entangled states.

Entanglement witnesses can be considered as geometric concepts: Due to the facts that the set of separable states S is convex and compact and the expectation value of an entanglement witness, as an observable, depends linearly on the state, $\mathcal{W}_{opt}$ defines a hyperplane in the set of all states. This hyperplane separates S from the set of entangled states, as visualized in fig. 3.4.1 below. In other words, $\mathcal{W}_{opt}$ forms a tangent plane to the set of separable states, and there exists (at least) one separable state $\tilde{\rho}_{sep} \in S$ such that $Tr(\mathcal{W}\tilde{\rho}_{sep}) = 0$. Using the definitions given by the inequalities above, one can say that all separable states are located on the side where $Tr(\mathcal{W}\rho) \geq 0$ holds, while $Tr(\mathcal{W}\rho) < 0$ covers the region of entangled states detected by the witness $\mathcal{W}$. That is the way how entanglement is detected in this thesis:

After constructing the witnesses, we identify the entangled states by showing the negative expectation value of the witness, $Tr(\mathcal{W}\rho) = \langle \mathcal{W} \rangle_\rho < 0$.

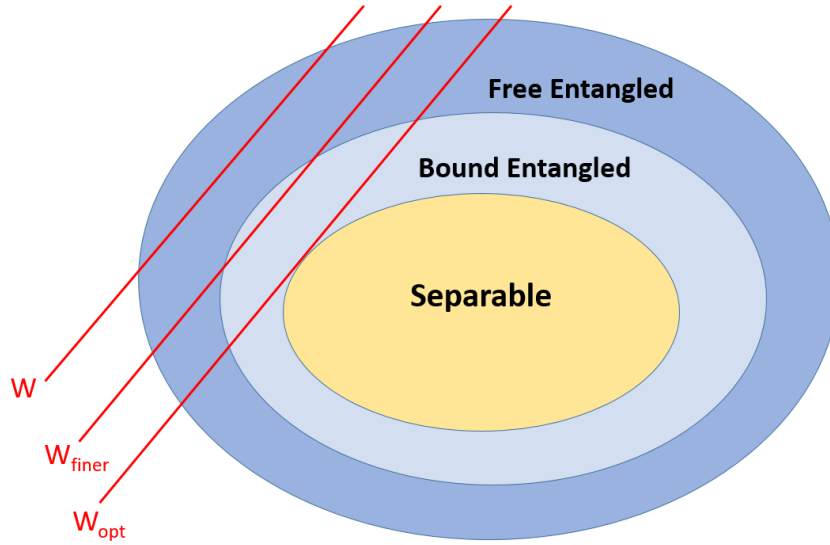


Figure 3.4.1: Schematic illustration of the set of all states in bipartite systems composed of the set of separable states, PPT bound entangled states and free (NPT) entangled states. The red lines correspond to different (linear) entanglement witnesses: While the witness $\mathcal{W}$ is just able to detect some free entanglement, $\mathcal{W}_{finer}$ is clearly more efficient than $\mathcal{W}$ and can thus detect more entanglement. However, no witness is finer than the hyperplane $\mathcal{W}_{opt}$, the optimal witness - even touching the set of separable states, segregating it from the entanglement section.

In order to guarantee the authenticity of the created witness one has to ensure that its expectation value is positive definite for all separable states, i.e. $Tr(\mathcal{W}\rho_{sep}) \geq 0$. This essential property is checked via a certain Wolfram Mathematica package [32] which is based on the composite parameterization of unitary groups [33, 34]. That file allows for the verification of the entanglement witnesses by first applying them to an arbitrary separable state ρ_{sep} and then employing all possible local unitary transformations U in order to cover all separable states:

$$Tr(\mathcal{W} \cdot (U_1 \otimes U_2)\rho_{sep}(U_1^\dagger \otimes U_2^\dagger)) \geq 0 \quad (3.17)$$

for all $U_1, U_2 \in \mathcal{U}(d)$ where $\mathcal{U}(d)$ marks the unitary group in the d -dimensional complex Hilbert space $\mathcal{H} = \mathbb{C}^d$.

Consequently, if one tries to minimize eq.(3.17) and obtains zero as a result (or actually a very small number close to zero) then one can be sure that $\mathcal{W}$ is a true entanglement witness. This check has been performed for all witnesses treated in this thesis.

Obviously, entanglement witnesses and in particular optimal witnesses can be very useful and are therefore very common in quantum information theory and experiments. In principle, one can detect all entangled states by witnesses. But the real problem is how to construct them and apply them to a specific problem. There are many ways of how to create geometrically

first an entanglement witness and then improve it to an optimal witness. In this work we will focus on two methods: Mutually Unbiased Bases (MUBs) and Symmetric Informationally Complete Positive Operator-Valued Measures (SIC-POVMs) - see sections 4.3 and 5.3.

When constructing entanglement witnesses one has to consider the so-called Choi-Jamiołkowski isomorphism [25, 26]: This isomorphism describes in general the connection between quantum states and positive maps. Two of its consequences are the relation between entanglement witnesses and positive but not completely positive maps and the association between decomposable witnesses and decomposable maps. We call an entanglement witness decomposable if we can write it in the form $\mathcal{W} = A + B^\Gamma$ where $A, B \geq 0$ and Γ marks the partial transpose operation with respect to one subsystem. Such a witness correlates with a decomposable, positive but not completely positive map, and thereby is not capable of detecting any bound entanglement. Consequently, we need witnesses relating to non-decomposable (positive but not completely positive) maps in order to find PPT entangled states.

4 Mutually Unbiased Bases

As already mentioned, we will try to detect the heavily mixed bound entangled states by utilizing entanglement witnesses constructed by mutually unbiased bases (MUBs). The first subchapter treats the notion of complementarity which is necessary in order to understand the concept of the mutual unbiasedness and then the definition and characteristics of MUBs. Subsequently, we consider the formation of MUBs by means of a certain method, the generalized Pauli matrices. After that we are ready to discuss the detection of entanglement via MUBs in the third subsection. This is done by exploiting a special criterion which we will call MUB-criterion since it is essential for the creation of MUB-entanglement witnesses.

4.1 Definition and properties of MUBs

In quantum physics, one often encounters observables that cannot be measured concurrently, i.e. they exclude each other. This special property is called complementarity and is crucial in quantum theory: Two observables are complementary if it is not possible to prepare a system such that the outcome of a measurement of both observables can be predicted with certainty [27]. Mathematically, this means that two complementary observables do not have a common eigenbasis.

Now, the idea of mutual unbiasedness carries the concept of complementarity to an extreme: If one knows precisely the measurement result of one observable (i.e. it is predictable with certainty) then the outcome of the complementary observable is completely unknown (that is every measurement yields a completely random value). In other words, if all eigenstates of the observable A have the same overlap with all eigenstates of the other observable B , then the eigenbasis of A and B can be described by a pair of mutually unbiased bases (MUBs). So, mathematically, the characteristic feature of MUBs can be expressed by the equal transition probabilities from each state of one MUB to all states of the other MUB, regardless of which pair of eigenvectors has been chosen [28].

Let us consider a set of orthonormal bases $\{B_k\}$ in the d - dimensional Hilbert space $\mathcal{H} = \mathbb{C}^d$ with $\{B_k\} = \{|i_k\rangle\}$ and $i = \{0, 1, \dots, (d-1)\}$. The bases $\{B_k\}$ are called mutually unbiased if and only if

$$p_{i_k, j_l} = |\langle i_k | j_l \rangle|^2 = \delta_{k,l} \delta_{i,j} + (1 - \delta_{k,l}) \frac{1}{d} = \underset{k \neq l}{=} \frac{1}{d}, \quad (4.1)$$

where p_{i_k, j_l} marks the transition probability from state $|i_k\rangle$ of the k^{th} MUB to state $|j_l\rangle$ of the l^{th} MUB for all $i, j = \{0, 1, \dots, (d-1)\}$.

So if we have a system that is prepared in a state of one of the MUBs, then a measurement performed in any state of another MUB reveals maximal incompatibility since we indeed do not gain any information via this measurement.

Due to these properties it is clear that MUBs are very useful in quantum information science, such as quantum state tomography, quantum error correction coding and in particular quantum key distribution - MUBs can be applied to many cryptographic protocols. But, as we will see, they can be also be employed on the detection of entanglement.

There are a lot of applications which involve a maximal set of MUBs, i.e. $(d+1)$ MUBs where d

is the dimension of the subsystem, since complete sets are informationally complete (essential in state tomography). However, so far, we only know that a complete set of MUBs does exist in prime and prime power dimensions. It is still unclear whether this holds in composite dimensions such as $d = 6, 10, 12, \dots$ as well. This great mathematical problem is known as the 'existence problem' or 'number problem'. On the other hand, it has been proven that for any dimension d there exist at least three MUBs which are formed by the eigenvectors of the generalized Pauli matrices σ_Z, σ_X and $\sigma_X \sigma_Z$. Numerical results indicate that for $d = 6$ there are indeed no more than these three MUBs.

Let us mention here that MUBs also play an important role in the study of entropic uncertainty relations since they maximize the lower bound of the uncertainty relation due to their maximal incompatibility. In fact, entropic uncertainty relations provide an alternative characterization of mutual unbiasedness (for a closer look at this issue, see [29]).

4.2 Construction of MUBs via Generalized Pauli Matrices

In order to detect bound entanglement as efficiently as possible we will only work with maximal sets of $(d+1)$ mutually unbiased bases. There are several ways of how to construct a complete set of MUBs, e.g. by using finite fields, Hadamard gates or the Heisenberg-Weyl group. In this thesis, MUBs are created via the Hadamard matrices which relate to the generalized Pauli matrices.

Hadamard matrices are unitary matrices that can be used to transform one MUB into each other. If one basis in a Hilbert space is the unit matrix, then all bases which are unbiased with respect to it can be represented by complex Hadamard matrices multiplied by a (dimensionally dependent) normalization factor. Generally, a Hadamard matrix H is written as

$$H = \sum_{i,j=0}^{d-1} \frac{1}{\sqrt{d}} e^{i\phi_{ij}} |i\rangle\langle j|, \quad (4.2)$$

where the phases ϕ_{ij} must be chosen such that H is unitary. The normalization factor $\frac{1}{\sqrt{d}}$ is crucial for this Hadamard matrix since it guarantees the creation of true MUBs (see eq.(4.1)). One of the most useful examples of H is the Fourier matrix since it works for any d . Consequently, by using the Fourier matrix we can always find a basis that is mutually unbiased relative to the standard basis. Choosing the phases $e^{i\phi_{ij}} = \omega^{-ij}$ with the root of unity $\omega = e^{\frac{2\pi i}{d}}$ we obtain the following Fourier matrix (discrete Fourier transformation)

$$H = \sum_{i,j=0}^{d-1} \frac{1}{\sqrt{d}} \omega^{-ij} |i\rangle\langle j|. \quad (4.3)$$

As one can see, there is a clear one-to-one correspondence between MUBs and Hadamard matrices: Finding a set of $d+1$ MUBs is equivalent to finding d Hadamard matrices. In order to form further bases that are unbiased with respect to both the standard basis and to the Fourier basis, i.e. the MUB created by applying the Fourier matrix to the standard basis, we need equivalent Hadamard matrices. This is done by e.g. multiplying the Fourier matrix from the left with a diagonal unitary matrix, or by permutations of rows and columns so that we can go from one Hadamard matrix to another one [30].

The Hadamard matrix in eq.(4.3) refers to the so-called generalized Pauli operators which are used to establish the MUBs for the bipartite qutrit system in this study:

$$\sigma_Z = \sum_{i=0}^{d-1} \omega^i |i\rangle\langle i| \quad (4.4)$$

$$\sigma_X = H \sigma_Z H^\dagger = \sum_{i=0}^{d-1} |(i+1 \bmod d)\rangle\langle i| \quad (4.5)$$

$$\sigma_X \cdot \sigma_Z = i \sigma_Y. \quad (4.6)$$

The generalized Pauli matrices are unitary, but not hermitian operators and satisfy the Weyl commutation rule [28]:

$$\sigma_X^m \sigma_Z^n = \omega^{-mn} \sigma_Z^n \sigma_X^m, \quad \forall m, n \in \mathbb{Z}. \quad (4.7)$$

This relation is the analogue of the identity $\sigma_Z \sigma_X = -\sigma_X \sigma_Z$ for the familiar Pauli operators σ_Z, σ_X in $d = 2$.

Analogous to $d = 2$ where a complete set of MUBs is attained by the three Pauli matrices σ_Z, σ_X and σ_Y , in any prime dimension the normalized eigenvectors of the following generalizations of Pauli operators can be used to create a full set of MUBs:

$$\sigma_X, \sigma_Z, \sigma_X \cdot \sigma_Z, \sigma_X \cdot \sigma_Z^2, \dots, \sigma_X \cdot \sigma_Z^{d-1}. \quad (4.8)$$

For the qutrit system in this work ($d = 3$) we obtain via that method of construction the following total set of MUBs:

$$\begin{aligned} B_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & B_2 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}, \\ B_3 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ \omega & \omega^2 & 1 \\ \omega & 1 & \omega^2 \end{pmatrix}, & B_4 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ \omega^2 & 1 & \omega \\ \omega^2 & \omega & 1 \end{pmatrix}. \end{aligned} \quad (4.9)$$

Although it is not relevant in this thesis, it should be mentioned here that forming MUBs in prime power dimensions is not as easy as in prime dimensions. That is because the Fourier matrix is no longer unique up to equivalences, e.g. in $d = 4$ there exists a one parameter family of inequivalent Hadamard matrices and one has to set the parameters properly in order to receive some additional MUBs [30]. Still, it is possible to create complete sets of MUBs in such dimensions by extending the method of construction via generalized Pauli operators, e.g. by making use of finite fields.

4.3 Entanglement Detection via MUBs

Now we want to try to connect the concept of complementarity and MUBs with the separability problem, i.e. how can we use MUBs in order to determine whether a given state is separable or entangled. In the following we will derive the MUB-criterion, i.e. a criterion that is satisfied by entanglement witnesses based on MUBs. The derivation of this criterion given here mainly refers to the paper by Spengler et al. in Ref. [27] where it was first established.

Let us consider a bipartite system composed of two d -dimensional subsystems, Alice and Bob, with their respective observables A and B . Thus, measurements on A or B will result in d different outcomes $\{0, \dots, d-1\}$. The correlations between these two observables can be quantified by constructing a correlation function C_{AB} for A and B which can be written as

$$C_{AB} = \sum_{i=0}^{d-1} \sum_{j=0}^{d-1} P_{AB}(i, j), \quad (4.10)$$

where $P_{AB}(i, j)$ describes the joint probability that a measurement on A yields the outcome i and on B the outcome j . Mathematically, the joint probability is given by

$$P_{AB}(i, j) = \langle i_A | \otimes \langle j_B | \rho | i_A \rangle \otimes | j_B \rangle, \quad (4.11)$$

where $\{|i_A\rangle\}$ and $\{|i_B\rangle\}$ represent the orthonormal bases relating to observable A and B and ρ denotes the state of the bipartite system.

The correlation function as the sum over all joint probabilities is also called the mutual predictability since it tells us the probability to determine the measurement result of one observable when knowing the outcome of the other one. If this probability is maximal, i.e. $C_{AB} = 1$ then the observables are fully correlated. But when the observables are completely uncorrelated the correlation function yields $C_{AB} = \frac{1}{d}$, that is the measurement results are completely random - measuring one observable does not bring us any information about the outcome of the other one.

Now let us relate the correlation function to the separability of a state. Therefore, we need at least another basis A' and B' in addition to A and B because only one set of measurement settings A and B cannot help us to distinguish between separable and entangled states: If we consider a maximally entangled pure state such as the Bell state $|\Omega_{00}\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i_A\rangle \otimes |i_B\rangle$ the correlation function obviously gives $C_{AB} = 1$ (this actually holds for all entangled pure states). But C_{AB} is also maximal for a classically correlated separable state $\rho_{CC} = \sum_{i=0}^{d-1} |\lambda_i|^2 |i_A\rangle \langle i_A| \otimes |i_B\rangle \langle i_B|$ with $\lambda_i \geq 0, \sum_i \lambda_i = 1$. So there is nothing we can learn about the separability of a state by using just one set of bases A and B . Now our previously defined mutually unbiased bases come into play. Let us consider the pure product state $|\psi_{sep}\rangle = |0_1\rangle \otimes |0_1\rangle$. If both observables A and B are measured in their own eigenbasis $\{|i_1\rangle\}$, the correlation function yields $C_{A_1 B_1} = 1$. But measured in another basis $\{|i_2\rangle\}$ that is mutually unbiased to $\{|i_1\rangle\}$, we obtain for the joint probability

$$\begin{aligned} P_{A_2 B_2}(i, i) &= Tr(|i_2\rangle \langle i_2| \otimes |i_2\rangle \langle i_2| |\psi_{sep}\rangle \langle \psi_{sep}|) = \langle i_2 i_2 | \psi_{sep} \rangle \langle \psi_{sep} | i_2 i_2 \rangle \\ &= |\langle i_2 | 0_1 \rangle|^2 \cdot |\langle i_2 | 0_1 \rangle|^2 = \frac{1}{d^2} \end{aligned} \quad (4.12)$$

and thus for the correlation function

$$C_{A_2 B_2} = \sum_{i=0}^{d-1} P_{A_2 B_2}(i, i) = \frac{1}{d}. \quad (4.13)$$

Thus, the two observables are completely uncorrelated due to the unbiasedness relation as it is expected for a separable state. So, the actual difference between entanglement and separability lies in the correlations in different basis choices.

We can then define the quantity $I_m = \sum_{k=1}^m C_{A_k B_k}$ as the sum over all correlation functions $C_{A_k B_k}$ where m denotes the number of MUBs that are used. For any pure product state like $|\psi_{sep}\rangle$ we obtain $I_m = 1 + \frac{m-1}{d}$ since in the first basis, the observables' eigenbasis, the mutual predictability is maximal while it is minimal for all the remaining $m - 1$ bases which are unbiased to the first one and to each other.

The quantity I_m is linear in the state $|\psi_{sep}\rangle\langle\psi_{sep}|$ - consequently, for any pure or mixed product state, that is for all separable states ρ_{sep} , the following condition holds:

$$I_m(\rho_{sep}) = \sum_{k=1}^m C_{A_k B_k} \leq 1 + \frac{m-1}{d}. \quad (4.14)$$

For the mathematical proof of this relationship, see Ref. [27]. Due to the fact that this upper bound is valid for all separable states when using m MUBs we will call this inequality the MUB-criterion. That criterion is essential in this thesis since any violation of eq.(4.14) indicates the detection of entanglement. In order to find bound entanglement we will work with a complete set of MUBs, i.e. $m = d + 1$ such that

$$I_{d+1}(\rho_{sep}) \leq 2 \quad (4.15)$$

will be our main condition to construct entanglement witnesses based on MUBs: We will use the quantity $2 - I_{d+1}$ to define a MUB-witness, and if the expectation value of the witness is negative (and thereby violating the MUB-criterion) it is clear that we have detected entanglement - in combination with the satisfied criteria for positivity and PPT we would even have bound entanglement. Let us remark at this point that it is not clear yet whether a full set of MUBs is necessary to detect bound entanglement. But in this study we want to reveal as much bound entanglement as possible, therefore, informational completeness given by all available MUBs for a certain dimension is required.

In Ref. [27] it is also shown that there cannot be more than $d + 1$ MUBs because, if so, we would have a great problem with detecting separability. Adding another MUB to the already existing $d + 1$ MUBs would end up detecting separable states as entangled ones. Hence, eq.(4.15) represents a direct connection between a complete set of MUBs in any dimension d and the upper bound on all separable states.

Recently, there have also been reports on the lower bounds for separable states with respect to MUBs [31]. While the upper bound is fixed for a maximal set of MUBs in every prime power dimension by eq.(4.15), the lower bound can change with d and the chosen set of MUBs, i.e. in certain dimensions such as $d = 4$ there can be a maximal and a minimal lower bound depending on different sets of m MUBs. However, in this thesis we will only consider the upper bound of separability via MUBs and (as we will see in the next chapter) via SICs.

Creating MUB-entanglement witnesses means that we have to take the MUB-criterion from inequality (4.15) into account but therefore we need to construct correlation functions utilizing the concept of MUBs to calculate the quantity I_{d+1} . This is done by reordering the MUB-vectors in Bob's subsystem, i.e. the second subsystem, which is achieved by applying Weyl operators to the MUBs. The Weyl matrices (explained in section 2.2) perform local shifts on the bases, reordering the basis vectors - but there are many ways to do that. Since each of the $d+1$ MUBs consists of d basis vectors, we have in general $(d+1)d!$ possibilities to rearrange the vectors, hence in our bipartite qutrit system $12! = 4.79 \times 10^8$ ways. It seems quite logical that it is impossible to handle all of them, indeed, we will just deal with some examples when constructing MUB-witnesses trying to detect bound entanglement. Many reorderings have been tested but those presented here have proven well-suited, partly owing to the results of a previous work on that topic (see Ref. [45]), and a few of them are random successes and/or surprises found by trial and error.

The following correlation function has been chosen for the making of our MUB-witnesses:

$$C_{A_k B_k} = \sum_{i=0}^{d-1} \text{Tr}(|b_i^k\rangle\langle b_i^k| \otimes (W_{lm}|b_i^k\rangle)^* (\langle b_i^k|W_{lm}^\dagger)^* \rho), \quad (4.16)$$

where $k = \{1, \dots, d+1\}$ enumerates the MUBs B_k , listed in (4.9), and $|b_i^k\rangle$ denotes the i -th basis vector $|b\rangle$ of the k -th MUB, W_{lm} marks the Weyl-operators with $l, m = \{0, \dots, d\}$ and ρ represents the state of the bipartite system. As one can see, the Weyl operators W_{lm} only reorder the vectors in one subsystem (we have chosen here the second one) so that we can establish correlations between the parties Alice and Bob.

Summing up the correlation functions and applying the MUB-criterion from eq.(4.15) yields the expectation value of our MUB-witness $\mathcal{W}$,

$$\langle \mathcal{W} \rangle_\rho = 2 - \sum_{k=1}^{d+1} C_{A_k B_k} = 2 - I_{d+1}(\rho), \quad (4.17)$$

that has to be non-negative, i.e. $\langle \mathcal{W} \rangle_\rho \geq 0$ for all separable states. This is checked via the Wolfram Mathematica package [32] that has been introduced in section 3.4, exploiting condition (3.17). It implements the composite parameterization of unitary groups which enables a checking for all separable states. All of the MUB-witnesses presented in this thesis have passed this efficient test, thus one can be sure that all of them are genuine entanglement witnesses. Finally after constructing and checking our witnesses we will optimize them to receive the optimal witness $\mathcal{W}_{opt}$ detecting the maximum possible amount of bound entanglement. For that purpose we will minimize the quantity $2 - I_{d+1}$ with respect to the parameters q_j , taking into account the constraints of positivity and PPT:

$$\langle \mathcal{W}_{opt} \rangle_\rho = \min_{q_j} \{2 - I_{d+1}(\rho(q_j)) | \rho(q_j) \geq 0, \rho^\Gamma(q_j) \geq 0\}, \quad (4.18)$$

where Γ denotes the partial transpose operation relating to one subsystem and ρ describes the state of the system.

One should note that the minimization calculation of the expectation values in eq.(3.17) and eq.(4.18) has been achieved for both MUB- and SIC-witnesses using the method "Random Search" for the *NMinimize*-command in Mathematica. It is the most effective tool, often

requiring a very large computation time (especially compared to the other methods available) but it cannot be fully excluded that the minimum found is not a global minimum but just a local one.

5 Symmetric Informationally Complete Positive Operator-Valued Measures

Now we are going to deal with the second form of entanglement witnesses that are considered in this thesis: the Symmetric Informationally Complete Positive Operator-Valued Measures, in short SIC-POVMs or just SICs as they are known in quantum information theory. We will treat this subject similar to MUBs in the chapter before. First, the idea behind SICs and the basics are covered. Thereafter we look at one technique of how to construct SICs because in general there are several ways to form a full set of them. The third subchapter deals with the usage of SICs for the construction of entanglement witnesses. It addresses the conditions which are necessary in order to detect any entanglement and ultimately bound entanglement via SICs. This will result in a criterion quite similar we have found for MUBs, that is why we will call it the SIC-criterion. Finally, we take a short look at the connection between MUBs and SICs which is given by the so-called quantum 2-designs. These are sets of quantum states that prove the equivalence of these two mathematical methods, and thereby allow a comparison of the entanglement witnesses created by them.

5.1 Definition and properties of SICs

To be able to deal with SIC-POVMs one has to take a look at POVMs in general. Quantum measurements mostly make use of positive operator valued measures (POVMs) since they represent a very generalized measurement. POVMs relate to the probabilities of the measurement results of an observable, thus they allow for an efficient description of the outcome statistics of a quantum measurement. That is why, in quantum theory, one often speaks of probability operator measurements (POMs) when actually POVMs are meant.

Mathematically, a POVM consists of positive operators E_m which have to satisfy the completeness condition $\sum_m E_m = \mathbb{1}$ otherwise the probabilities of the measurement results given by $\text{Tr}(E_m \rho)$ with ρ being the state of the system may not sum up to one. Physically, one can say that each POVM element in the set $\{E_m\}$ describes a possible result of measurement.

We call a POVM informationally complete (IC-POVM) if there are d^2 POVM elements E_m which are able to determine completely and thereby uniquely the state to be measured. This is because an unknown state can be described by $d^2 - 1$ parameters and in addition to that one has to consider the completeness relation. Consequently, exactly d^2 elements provide a minimal informationally complete POVM. Naturally, this is, e.g., of great interest in the field of quantum state tomography and if one wants to maximize the efficiency at determining the state, the d^2 POVM elements should be proportional to one-dimensional projectors, i.e. rank-one projectors [35].

Now, the symmetric informationally complete POVMs (SIC-POVMs) form a special set of POVMs. They can be defined as follows: Consider a set of exactly d^2 POVM elements E_m proportional to rank-one projectors P_m , i.e. $E_m \propto P_m = |\psi_m\rangle\langle\psi_m|$, with $P_m^2 = P_m$ and the normalized vectors $|\psi_m\rangle \in \mathbb{C}^d$, satisfying

$$\text{Tr}(P_m P_n) = \frac{1}{d+1}(1 + d\delta_{mn}) \quad (5.1)$$

for $m, n = \{1, \dots, d^2\}$. If this condition holds, the set of positive operators $\{E_m = \frac{1}{d}P_m\}_{m=1}^{d^2}$ is said to be a SIC-POVM. So, the POVM elements E_m themselves are not projectors due to the prefactor $\frac{1}{d}$. Equivalently, one could rewrite eq.(5.1) by just using pairs of the distinct unit vectors $|\psi_m\rangle$ such that

$$|\langle\psi_m|\psi_n\rangle|^2 = \frac{1}{d+1} \quad (5.2)$$

for $m \neq n$. Thus, the additional property 'symmetric' in combination with the other characteristics of SIC-POVMs is given by the fact that the squared inner products for any pair of distinct vectors are equal. Therefore, SIC-POVMs can also be seen as a (maximal) set of pairwise equiangular lines in the Hilbert space since the vectors $|\psi_m\rangle$ are evenly spaced.

SIC-POVMs or, for brevity, SICs are due to their qualities very interesting in quantum information science since they can serve as a so-called 'standard quantum measurement', especially in the field of research of quantum state tomography and quantum cryptography. Moreover, SICs also have applications for the technical side of foundational studies, in particular QBism (Quantum Bayesianism) which can be seen as a new, in a sense, 'subjective' interpretation of quantum theory, first introduced in 2010 [39, 40]. And, just like MUBs, SICs can be utilized for entanglement detection.

It should be mentioned here that it is still an open problem in mathematics whether SIC-POVMs exist in any finite dimension. So far, for all dimensions up to $d = 151$ and in some cases beyond that, up to $d = 1299$, exact solutions for SIC-POVMs are known. Numerical solutions to high precision have been found in even higher dimensions, up to $d = 2208$, by means of different numerical methods and exploiting new types of symmetry beyond the fundamental definition of SIC-POVMs [36–38]. But an analytical proof for the so-called Zauner's conjecture, i.e the existence of d^2 equiangular lines for arbitrary dimensions, is still lacking.

5.2 Construction of Hesse-SICs

Now we are going to construct a full set of SIC-POVMs using the Heisenberg-Weyl group. This will result in the establishment of the so-called Hesse-SICs. Since we only deal with bipartite qutrits in this thesis we will finally acquire $d^2 = 9$ Hesse-SICs that can be used to seek bound entanglement just as the full set of $d + 1 = 4$ MUBs in an analogous way.

But first we want to take a closer look at the geometric structure of the SICs. In general, giving an appropriate visualization of these structures is quite intricate, in particular in higher dimensions. But in the case of qubits ($d = 2$) it is easy to find a good match: The four SIC states represent the vertices of a regular tetrahedron within the Bloch sphere and can be written in the following way [31]:

$$\begin{aligned} |s_1\rangle &= |0\rangle, \\ |s_2\rangle &= \frac{1}{\sqrt{3}}(|0\rangle + \sqrt{2}|1\rangle), \\ |s_3\rangle &= \frac{1}{\sqrt{3}}(e^{-\frac{i\pi}{3}}|0\rangle + \sqrt{2}e^{\frac{i\pi}{3}}|1\rangle), \\ |s_4\rangle &= \frac{1}{\sqrt{3}}(e^{\frac{i\pi}{3}}|0\rangle + \sqrt{2}e^{-\frac{i\pi}{3}}|1\rangle), \end{aligned} \quad (5.3)$$

where $|0\rangle$ and $|1\rangle$ label the standard basis for $\mathbb{C}^2$ and the SIC-vectors $\{|s_m\rangle\}_{m=1}^4$ have to satisfy condition (5.2).

Generally, most SICs are created using an additional type of symmetry. This is the so-called group covariance: Finding a single vector that is known as the fiducial vector $|\psi_f\rangle$ and applying d^2 unitary representations $\{U_g\}$ on $\mathbb{C}^d$ to it allows us to form the SIC-POVM P . To do this, it is necessary that the following conditions are satisfied [13]:

- For any SIC-vector $|\psi_m\rangle \in P$ and any U_g being an element of a group G , i.e. $U_g \in G$, it holds $U_g|\psi_m\rangle \in P$, so P does not change under any unitary U_g
- For any $|\psi_m\rangle, |\psi_n\rangle \in P$, there exists a U_g such that $U_g|\psi_m\rangle = |\psi_n\rangle$, so the SIC-POVM is constituted by the group action $P = \{U_g|\psi_f\rangle\}$ where $|\psi_f\rangle$ denotes the normalized fiducial vector.

That procedure of generating SICs is also called taking the orbit of a fiducial vector. The most commonly used construction method of SICs is the group covariance under the group $\mathbb{Z}^d \times \mathbb{Z}^d$, in particular the Weyl–Heisenberg group. This group is established by the Weyl operator, see eq.(2.7), which combines the phase operator Z and the cyclic shift operator X . They can be written in the form

$$Z|j\rangle = \omega^j|j\rangle \quad (5.4)$$

$$X|j\rangle = |(j+1) \bmod d\rangle, \quad (5.5)$$

where $\omega = e^{\frac{2\pi i}{d}}$ marks the root of unity and $\{|j\rangle\}_{j=0}^{d-1}$ describes the computational basis of $\mathbb{C}^d$. These two operators comply with the Weyl commutation relation,

$$X^a Z^b = \omega^{-ab} Z^b X^a \quad (5.6)$$

with $a, b = \{0, \dots, d-1\}$. One can see that X and Z almost, up to a phase factor, commute but they do not.

Now we can define the Heisenberg-Weyl displacement operators [36]:

$$D_{ab} = (-e^{i\pi/d})^{ab} X^a Z^b. \quad (5.7)$$

Thus, the Heisenberg-Weyl SICs are given by

$$|s_{a,b}\rangle = (e^{-iab\pi/d}) X^a Z^b |\psi_f\rangle. \quad (5.8)$$

One should note here that it is not clear yet whether a SIC has to be group covariant in general. But it has already been shown that in prime dimensions, each SIC-POVM is covariant with respect to at least one Heisenberg–Weyl (HW) group [41].

Let us demonstrate some examples for the fiducial vector. For $d = 2$ we have

$$|\psi_f\rangle = \frac{1}{\sqrt{6}}(\sqrt{3+\sqrt{3}}|0\rangle + e^{\pi i/4}\sqrt{3-\sqrt{3}}|1\rangle). \quad (5.9)$$

Applying the upper method in order to construct Heisenberg-Weyl SICs we yield the four states displayed in (5.3). Now let us move to the crucial case for this thesis: $d = 3$. Considering qutrits, we do not have a unique Heisenberg–Weyl group as we have for qubits. Instead, each

(group covariant) SIC-POVM may be covariant with respect to three or even nine Heisenberg-Weyl groups [41]. Moreover, we remarkably encounter several additional, more subtle, symmetries apart from group covariance in this dimension. One example of Heisenberg-Weyl SIC-POVMs for qutrits is the orbit of the following fiducial vector

$$|\psi_f^{(Hesse)}\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle). \quad (5.10)$$

Employing this vector we can create the so-called Hesse-SICs which have been utilized to render all the results concerning SICs presented in this work. Therefore the full set of Hesse-SICs $\{|s_n\rangle\}_{n=1}^9$ is displayed here (in the order they have been used throughout) [31]:

$$\begin{aligned} |s_1\rangle &= \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), \\ |s_2\rangle &= \frac{1}{\sqrt{2}}(\omega|1\rangle - \omega^2|2\rangle), \\ |s_3\rangle &= \frac{1}{\sqrt{2}}(\omega^2|1\rangle - \omega|2\rangle), \\ |s_4\rangle &= \frac{1}{\sqrt{2}}(-|0\rangle + |2\rangle), \\ |s_5\rangle &= \frac{1}{\sqrt{2}}(\omega|0\rangle - |2\rangle), \\ |s_6\rangle &= \frac{1}{\sqrt{2}}(-\omega^2|0\rangle + |2\rangle), \\ |s_7\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle), \\ |s_8\rangle &= \frac{1}{\sqrt{2}}(\omega^2|0\rangle - |1\rangle), \\ |s_9\rangle &= \frac{1}{\sqrt{2}}(\omega|0\rangle - |1\rangle), \end{aligned} \quad (5.11)$$

where $\omega = e^{\frac{2\pi i}{3}}$ and $|0\rangle$, $|1\rangle$ and $|2\rangle$ indicate the standard basis for $\mathbb{C}^3$.

The name 'Hesse' derives from the link between these SIC vectors and the Hesse configuration in the complex projective plane which is a well-known structure in algebraic geometry (design theory) [42, 43].

5.3 Entanglement Detection via SICs

Analogous to chapter 4.3 we will now establish a separability criterion for SIC-POVMs, i.e. a condition in terms of an inequality that must be violated by a collection of SICs in order to detect entangled states. Therefore this SIC-criterion for the construction of SIC-entanglement witnesses will look quite similar to the one satisfied by MUB-witnesses and is yet different.

Since the derivation of the upper bound for all separable states exploiting SICs is in principle the same we have already done using MUBs - as we apply in both cases the concept of complementarity to the separability problem - we will only summarize here its most important relations and results and, in particular, stress the differences compared to the MUB-version

explained in 4.3.

We start again with the correlation function C_{AB} for our observables A and B but this time we construct C_{AB} via SICs and thereby have to take eq.(5.2) into account. This condition guarantees the equivalence of any pair of elements to any other pair because the pairwise inner products always provide a constant value (compare to the MUB-condition (4.1)). So, if A and B share the pure product state $\rho = |0_1 0_1\rangle\langle 0_1 0_1|$ and apply measurements from a set of SICs we receive the following correlation function

$$C_{A_2 B_2} = \text{Tr}(|s_2\rangle\langle s_2| \otimes |s_2\rangle\langle s_2| \rho) = \frac{1}{(d+1)^2}, \quad (5.12)$$

where $\{|s_k\rangle\}_{k=1}^m$ denote the SIC-vectors which are here, for simplicity, the same for the sub-systems A and B . Again, as before with MUBs, $C_{A_1 B_1} = 1$ since we can always choose the observable's eigenstates as appropriate SIC-states in order to optimize this protocol exploiting complementarity.

Then we can bring another quantity I_m which is given by all correlation functions $C_{A_k B_k}$ in total. Therefore, I_m can be seen as the collection of probabilities when the measurement operators of m SICs are applied to ρ :

$$I_m(\rho) = \sum_{k=1}^m C_{A_k B_k} = 1 + \frac{m-1}{(d+1)^2}. \quad (5.13)$$

Hence, for all separable states ρ_{sep} , pure and mixed, we obtain an upper bound

$$I_m(\rho_{sep}) \leq 1 + \frac{m-1}{(d+1)^2}. \quad (5.14)$$

Since only full sets of SICs are used in this study we can set $m = d^2$ and attain finally our SIC-criterion

$$I_{d^2}(\rho_{sep}) \leq \frac{2d}{d+1}. \quad (5.15)$$

One can recognize here an important difference between the SIC-criterion and the MUB-criterion: While the upper bound on all separable states is independent of the dimension d for a complete set of MUBs (see condition 4.15), it is not with respect to a total set of SICs. Instead, the upper bound value of the SIC-criterion increases with d : for qutrits it yields $3/2$ but it is $8/5$ for $d = 4$ and already $5/3$ for $d = 5$; it obviously approaches (asymptotically) the unchanging value of the MUB-criterion: $I_{d+1}(\rho_{sep}) = 2$. Hence, for a SIC-POVM the upper criterion looks differently in every dimension.

Let us note here that for SICs, just as for MUBs, lower bounds for all separable states in addition to the upper bounds have lately been found [31]. Thus, the expectation value of the MUB- or SIC-entanglement witness must lie within a certain interval to prove a state to be separable. However, if one does not use a complete set of SIC-POVMs, both bounds become dependent on the number of chosen SICs. Moreover, in $d = 3$ and maybe in every dimension $d > 2$, measurements taken from a set of SICs can result in a minimal and maximal lower and upper bound, respectively. This seems another distinction from MUBs: As far as we know, the upper bound of the MUB-criterion is always fixed for a total set of MUBs, independent of the dimension d . And even if less than $d + 1$ bases are employed, the upper bound just depends

on d and the number of MUBs used, but there is not a maximal or minimal upper bound. Considering the lower bound of MUBs, however, that changes: This bound on separable states varies, depending on d and the choice of the bases, i.e. the specific set of MUBs, providing a maximal and a minimal lower bound on MUBs, at least for $d > 3$ [31]. These are some very interesting and surprising insights into the structure of MUBs and SICs but here we will only cover the upper bound and full sets of bases and measurement operators.

So far we have discussed all necessary properties an entanglement witness constructed by means of SIC-POVMs has to satisfy. Now we want to explicitly create such a witness by applying a similar technique we have used for the generation of MUB-witnesses before. We will use again Weyl operators to form proper correlation functions between the observables in our bipartite system. The operators are employed on the SICs in one of the subsystems - referring to the MUB-case before, we choose once more Bob's party - causing local shifts of the SIC-vectors and thereby reorder them.

Due to the fact that we always make use of a full set of SICs, we have in total $d^2!$ possibilities to rearrange the vectors. Again, as with MUBs, a great many of these realignments have been tested to construct useful SIC-witnesses. Only those yielding the best results which could have been found are considered here. Some Weyl operators have been applied to both MUBs and SICs for comparison purposes, e.g., for the construction of MUB/SIC-witnesses the operator W_{01} from (2.14) is first applied to the first MUB and afterwards to the first SIC-vector. Then one can compare which witness is able to detect entanglement, ideally bound entanglement, more efficiently. However, there is also some SIC-shifting presented here that is achieved by Weyl matrices which have not been used on MUBs, and vice versa, because they only yield remarkable results when applied either to MUBs or to SICs.

Due to the reasons explained above the correlation function for the generation of SIC-witnesses reads as follows:

$$C_{A_k B_k} = \text{Tr}(|s_k\rangle\langle s_k| \otimes (W_{lm}|s_k\rangle)^* (\langle s_k|W_{lm}^\dagger)^* \rho), \quad (5.16)$$

where $k = \{1, \dots, d^2\}$ enumerates the SIC-POVM elements and correlation functions, $|s_k\rangle$ gives the k -th SIC-vector, W_{lm} the Weyl operators with $l, m = \{0, \dots, d-1\}$ and ρ denotes the state of the bipartite system.

Now, one could think that, in complete analogy to the derivation of MUB-witnesses, for the construction of SIC-witnesses $\mathcal{W}$ these correlation functions are summed up and then the SIC-criterion (5.15) for $d = 3$ is exploited:

$$\langle \mathcal{W} \rangle_\rho = \frac{3}{2} - \sum_{k=1}^{d^2} C_{A_k B_k} = \frac{3}{2} - I_{d^2}(\rho). \quad (5.17)$$

If that was true, the expectation value of any SIC-witness would have to be positive definite, i.e. $\langle \mathcal{W} \rangle_\rho \geq 0$, for all separable states. This is checked via the same Wolfram Mathematica package [32] that has already been used for the examination of the MUB-witnesses (see condition (3.17)). All of those have successfully performed the validation, confirming that for a full set of MUBs the upper bound value on the set of separable states is always 2.

However, during this procedure of verification, it has been found out that local shifts on SIC-vectors, implemented by Weyl operators, mostly change the upper bound of SIC-witnesses. While the first Weyl operator $W_{00} = \mathbb{1}$ clearly does not shift anything, for both W_{01} or W_{02}

applied to the first or any other SIC-vector $|s_n\rangle$, $n = \{1, \dots, 9\}$, in Bob's subsystem, the upper bound for all separable states has the value $15/8$. But if both Weyl-shifts are utilized, e.g. W_{01} acting on the first SIC $|s_1\rangle$ and W_{02} on the second one $|s_2\rangle$, then the calculation of the upper bound yields 1.94075. Obviously, using local Weyl shifts to generate SIC-witnesses means that the upper bound has to be computed for every SIC-witness individually, and thus the SIC-criterion adapted. Hence, eq.(5.17) does not generally hold - it has to be corrected for each new combination of Weyl operators employed on the SIC-vectors in eq.(5.16), e.g., for W_{01} applied to $|s_1\rangle$ we have

$$\langle \mathcal{W} \rangle_\rho = \frac{15}{8} - \sum_{k=1}^{d^2} C_{A_k B_k} = \frac{15}{8} - I_{d^2}(\rho). \quad (5.18)$$

Utilizing the same Weyl operator onto each SIC-vector in Bob's subsystem such as W_{01} or W_{02} applied to all Hesse-SICs, i.e. reordering all of Bob's SIC-vectors concurrently, really provides $\frac{3}{2}$ as its correct upper bound - the same holds for some special combinations like W_{02} on $|s_1\rangle$ and W_{01} on $|s_4\rangle$, or W_{01} on $(|s_1\rangle, |s_4\rangle)$ and $|s_7\rangle$). But if less than d^2 Weyl operators W_{kl} are applied, meaning that there is at least one SIC onto which no operator works, or if not the same W_{kl} covers all the SICs, then the upper bound starts to vary.

In fact, this is an essential result that just holds for SICs but not for MUBs. Concerning MUB-witnesses the upper bound never has to be adjusted regardless of whether the Weyl matrices are only applied to single bases (local shifts) or to all MUBs. Hence, it is imperative that all the SIC-witnesses put to use for detection of entanglement are checked, and their upper bound on the set of separable states by means of eq.(3.17) individually calculated. This procedure has been carried out for all SIC-witnesses studied here in order to guarantee genuine entanglement witnesses.

Lastly we will optimize the entanglement witness in order to obtain the most efficient, i.e. the optimal one, denoted by $\mathcal{W}_{opt}$, which is capable of detecting the maximum amount of entanglement and thereby increase the chance to cover bound entanglement. Following similar considerations based on MUBs before, we will minimize the expectation value of the SIC-witness with respect to the parameters q_j , taking into account the constraints of positivity and PPT. As an example, optimizing the witness realized by W_{01} applied to $|s_1\rangle$ in eq.(5.18) gives

$$\langle \mathcal{W}_{opt} \rangle_\rho = \min_{q_j} \left\{ \frac{15}{8} - I_{d^2}(\rho(q_j)) \mid \rho(q_j) \geq 0, \rho^\Gamma(q_j) \geq 0 \right\}, \quad (5.19)$$

where Γ denotes the partial transpose operation relating to one subsystem and ρ describes the state of the bipartite system. Again, computation of the minimum expectation value has been implemented by the method "Random Search" for the *NMinimize*-command in Mathematica.

5.4 Equivalence between MUBs and SICs: Quantum 2-designs

Before we attend to the last chapter about the magic simplex and the different families of states located within there, we want to look more closely at the relationship between MUBs and SICs. Complete collections of MUBs and SICs are so-called quantum 2-designs, thus, if less than $d + 1$ MUBs or less than d^2 SICs are used (or available), they are considered as

subsets of a quantum 2-design. In general, a quantum k -design is defined in the following way:

A set of pure quantum states $\{|\psi_m\rangle\} \subseteq \mathbb{C}^d$ is said to be a quantum k -design if the average value over the set for polynomials of degree k or less is identical to the average over all normalized states via the Haar measure [31]. In other words, a quantum k -design can be seen as a probability distribution over pure quantum states $\{|\psi_m\rangle\} \subseteq \mathbb{C}^d$ with probability p_m that has the same properties as the probability distribution over the Haar measure on unit vectors for polynomials of degree k or less, thus

$$\sum_m p_m (|\psi_m\rangle\langle\psi_m|)^{\otimes k} = \int (|\psi\rangle\langle\psi|)^{\otimes k} d\psi. \quad (5.20)$$

The Haar measure is related to an invariant volume dU_C , i.e. a volume which does not change under any unitaries U_1, U_2 ,

$$dU_C = d(U_1 U_C) = d(U_C U_2). \quad (5.21)$$

A well-known example of the Haar measure is the Jacobian determinant. Since we are only interested in quantum 2-designs the integral over the Haar measure for $k = 2$ is given by

$$\int (|\psi\rangle\langle\psi|)^{\otimes 2} d\psi = \int_{\mathcal{U}} (U \otimes U |\psi\rangle\langle\psi| U^\dagger \otimes U^\dagger) dU = \Pi_{sym}, \quad (5.22)$$

where $\mathcal{U}$ represents the unitary group and Π_{sym} denotes the projector onto the symmetric subspace of $\mathbb{C}^d \otimes \mathbb{C}^d$,

$$\Pi_{sym} = \frac{1}{2}(\mathbb{1}_d \otimes \mathbb{1}_d + dP_{00}^\Gamma), \quad (5.23)$$

where P_{00} indicates a maximally entangled state and Γ the partial transpose operation.

Hence the quantum 2-design can be written as

$$\frac{1}{n} \sum_{m=1}^n (|\psi_m\rangle\langle\psi_m|)^{\otimes 2} = \frac{2}{d(d+1)} \Pi_{sym}. \quad (5.24)$$

This results in an important relationship between MUBs and SICs. The quantum 2-design can be decomposed into a full set of $(d+1)$ MUBs or d^2 SICs [31]:

$$\frac{2}{d(d+1)} \Pi_{sym} = \frac{1}{d(d+1)} \sum_{k=1}^{d+1} \sum_{i=0}^{d-1} (|b_i^k\rangle\langle b_i^k|)^{\otimes 2} = \frac{1}{d^2} \sum_{m=1}^{d^2} (|s_m\rangle\langle s_m|)^{\otimes 2}, \quad (5.25)$$

where $|b_i^k\rangle$ is the i -th basis vector $|b\rangle$ of the k -th MUB and $|s_m\rangle$ denotes the m -th SIC-vector. One can interpret eq.(5.25) in such a way that the total information can be used either by a total set of MUBs or a total set of SICs, indicating the equivalence of these two methods.

However, one should notice that, if Weyl operators are applied to MUBs and SIC-vectors in order to implement local shifts for the detection of bound entanglement one cannot consider MUBs and SICs as quantum 2-designs any more. Hence, the equivalence between MUBs and SICs (even for a full set) may not be given any more as well.

Moreover, it still poses a riddle why a complete set of SICs seems to exist for each dimension d but it apparently does not for MUBs despite the relationship in (5.25), e.g. for $d = 6$. It has been shown that k -designs such as MUBs or SICs do exist in all dimensions but the problem is that it is generally not known how to create them for an arbitrary d .

6 Comparing Bound Entanglement Detection: MUBs vs. SICs

In search of bound entanglement, the entanglement witnesses we have constructed via MUBs and SICs are now applied to several bipartite qutrit families of states which lie in the magic simplex. This special subspace of the state space is defined and explained first, then we start to investigate the classes of states dependent on the number of parameters they are based on, starting with the smallest number. During the work on that thesis many different families of states have been checked but in most of them no or almost none bound entanglement has been found, regardless of the witness employed on them. But in a few cases we have been successful and able to provide requested and sometimes very remarkable results. Most of them will be listed in several tables to guarantee an appropriate comparison of the output data between different witnesses and families of states. This makes it clear which MUB- and SIC-witnesses are more efficient than others and which are the most powerful ones. Afterwards the outcomes are analyzed and discussed in great detail. Furthermore, to make this quite abstract matter more vivid, we will graphically visualize the findings of some chosen witnesses, e.g., for comparison purposes between different MUB- and SIC-witnesses and in particular if it comes to the discovery of bound entanglement. An overview of all the important results rendered and discussed here is provided in the overall table 7.0.1 on page 63.

6.1 The Magic Simplex

Mathematically, a simplex is the simplest form of a polytope. An n -simplex is an n -dimensional polytope with $n + 1$ vertices, e.g. a 2-simplex is given by a triangle while the tetrahedron represents a 3-simplex. In general, an n -simplex can be defined using $n+1$ affinely independent points $x_0, x_1, \dots, x_n \in \mathbb{R}^n$ in the Euclidean space such that

$$\mathfrak{W}^{(n)} = \{p_0x_0 + p_1x_1 + \dots + p_nx_n \mid p_i \geq 0, \sum_{i=0}^n p_i = 1\}. \quad (6.1)$$

Thus, all of the points within the simplex can be seen as a mixture - a convex combination to be precise - of the pure points $\{x_i\}_{i=0}^n$ spanning the simplex.

Now, a magic simplex can be described as a convex combination of all d^2 mutually orthogonal maximally entangled states. Without loss of generality, one can choose those states to be the Bell states $|\Omega_{kl}\rangle$ which have already been defined in eq.(2.13) for the bipartite case. To each of them we will associate a projection operator P_{kl} given by

$$P_{kl} = |\Omega_{kl}\rangle\langle\Omega_{kl}|, \quad (6.2)$$

which describes the density matrix for the Bell state $|\Omega_{kl}\rangle$. The pure states P_{kl} span the geometrical object of our interest and mark its d^2 corners. Therefore, the magic simplex $\mathfrak{W}$ is defined as the convex combination of all Bell states [15]:

$$\mathfrak{W} = \left\{ \sum_{k,l=0}^{d-1} c_{kl} P_{kl} \mid c_{k,l} \geq 0, \sum_{k,l=0}^{d-1} c_{k,l} = 1 \right\}. \quad (6.3)$$

The magical simplex is a $d^2 - 1$ subspace in the d^2 Euclidean space that displays all locally maximally mixed states, i.e. the reduced matrices (partial trace with respect to one subsystem) of the states are maximally mixed. In other words, this simplex covers all the states which have maximally mixed subsystems since its vertices are the maximally entangled states. The maximally mixed state is located at the origin of the simplex. While for qubits the magic simplex forms a tetrahedron spanned by the four mutually equally distant Bell states, for qutrits $\mathfrak{W}$ is an 8-dimensional object - a 'generalised tetrahedron' - in the 9-dimensional Euclidean space which can naturally no longer be visualized or imagined. But this is not necessary anyway due to the properties of the magic simplex.

The reason why this simplex is that useful is its high symmetry. Since Weyl operators that are used to construct the Bell states P_{kl} and thereby the vertices of the simplex, compose a discrete group, $\mathfrak{W}$ can be significantly simplified [6, 44]: There are some mixtures of P_{kl} which are geometrically equivalent, e.g. they have the same geometry with regard to separability and entanglement and therefore bound entanglement as well. Hence, it is not necessary to examine all possible combinations of P_{kl} because many of them belong to the same equivalence class. In fact, the set of index pairs (k, l) defines a discrete classical phase space where l gives the coordinate in the position space and k relates to the momentum space. Each point (k, l) can be associated with one of the Bell states P_{kl} . Such a phase space structure for bipartite qutrits is shown in figure 6.1.1. If one applies a Weyl operator to any P_{kl} one can transform one Bell state into another one. But if the same local unitary transformation is employed on one Bell state d times one receives the original state due to the group structure of the Weyl operators. Thus, these three Bell states, e.g. P_{00}, P_{10} and P_{20} or P_{00}, P_{11} and P_{22} , create a phase space line. For bipartite qutrits there are four non-parallel lines which are red-coloured in fig. 6.1.1, where P_{00} is our starting point. To each of those lines we can assign three parallel lines, so, all in all, there are $(d+1)d$ phase space lines for dimension d showing the same geometry, i.e. for qutrits we obtain 12 lines.

These line states are very important since they represent the twelve separable states that are furthest from the origin of the simplex, thus the outmost separable states in $\mathfrak{W}$ [15]. They are given by

$$\rho_{line} = \frac{1}{d} \sum_{(k,l) \in line} P_{kl}. \quad (6.4)$$

One can only generate such separable line states by equally mixing all Bell states on a line, such as $\frac{1}{d} \sum_{k=0}^{d-1} P_{k0}$. Mixing just two (out of three) Bell states on a line or adding another Bell state which does not belong to the same line results in an entangled state.

Another characteristic of the magic simplex are the already discussed isotropic states, see (3.3). These mixtures of Bell states and the globally maximally mixed state connect the corners of the simplex with its center. Therefore, the isotropic witness displays the optimal entanglement witness for any Bell state.

If we consider again qubits, the four Bell states generate a tetrahedron as the magic simplex and partial transposition of them create another tetrahedron but an inverted one. The intersection of these two objects constitutes an octahedron (a double pyramid) which covers all of the PPT states. Since the PPT criterion is necessary and sufficient for $d = 2$, this octahedron represents a subset of separable states $S \cap \mathfrak{W}$ where S is the set of all separable states. Finding the analogue to the octahedron of qubits for the bipartite qutrit case is not that easy. For an 8-dimensional simplex this region cannot be graphically visualized by a simple geometrical

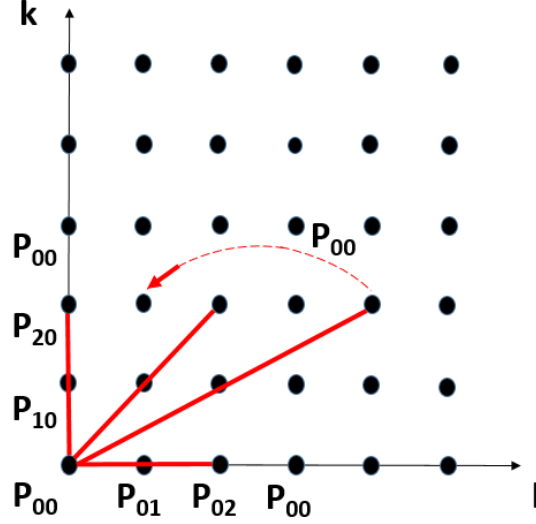


Figure 6.1.1: Discrete classical phase space structure of the magic simplex for bipartite qutrits ($d = 3$). Each point (k, l) corresponds to a Bell state P_{kl} . In this drawing four completely equivalent squares, each consisting of nine Bell states, are given where the red lines mark the four non-parallel lines beginning from P_{00} at the origin - the other P_{00} 's are supposed to show the starting points of the other cells for the sake of clarity. We can find three parallel lines to each red line, resulting in 12 unitary equivalent phase space lines, i.e. they reveal the same geometry with respect to separability and entanglement.

object, instead, one needs to define two polytopes in order to understand separability in a higher dimensional magic simplex:

First, we construct the so-called kernel polytope $\mathcal{K}$ which is composed of all the convex combinations of the twelve line states we have explained in eq.(6.4). It is given by

$$\mathcal{K} = \left\{ \sum_{\text{lines } a} p_a \rho_{\text{line } a} \mid p_a \geq 0, \sum_a p_a = 1 \right\}, \quad (6.5)$$

where *lines* a enumerates the twelve lines. Hence the kernel polytope is a region completely made up of separable states.

The other one is the enclosure polytope $\mathcal{E}$ that can be mathematically described by

$$\mathcal{E} = \{c_{kl} \mid \text{all } c_{kl} \in [0, \frac{1}{d}]\}. \quad (6.6)$$

The enclosure polytope is a wider and more general object than the kernel polytope, in fact $\mathcal{E}$ comprises $\mathcal{K}$, and it has the same geometrical symmetries as the magic simplex. We find that all states inside of the kernel polytope are separable and all states outside of the enclosure polytope are entangled. While for qubits those two regions are identical - which is why there is no bound entanglement at all for $d = 2$ - their differentiation is crucial when we move on to higher dimensions such as $d = 3$. In the region between $\mathcal{E}$ and $\mathcal{K}$, i.e. outside of $\mathcal{K}$ but inside of $\mathcal{E}$, there are PPT states that can be separable but they do not have to be. Consequently,

this is the zone where bound entangled states are most probable to find in the simplex since all the necessary conditions are satisfied: positivity, positive partial transpose and it is the region next to the kernel polytope, the set of separable states. So when investigating our families of states we are particularly interested in that area.

However, it should be mentioned here that for all dimensions $d > 2$, the magic simplex is no longer unique as it is for qubits, i.e. there exist locally maximally mixed states which cannot be assigned to the simplex. Hence, they lie outside of $\mathfrak{W}$, in other words, they cannot be diagonalized with the maximally entangled states, the Bell states. But even if the latter holds, this does not mean that those states can be embedded into $\mathfrak{W}$. Moreover, it has been shown that there exist complete sets of d^2 mutually orthogonal Bell states which do not establish a unitary equivalent version of the magic simplex. This new simplex might have geometrical properties that are quite different from the one explained above.

6.2 Families of States

In the following subsections we will address several bipartite qutrit families of states characterized by different parameterizations within the magic simplex. Several MUB- and SIC-witnesses will then be applied to them trying to detect as much bound entanglement as possible. Those classes of states can generally be seen as an extension of the class of isotropic states, see eq.(3.3), with more than one Bell projector and more than one parameter. The parameters are supposed to weight the Bell states individually or treat an entire phase space line; they might also be the coefficients for more than one line.

In general, the nine Bell projectors are distributed among different numbers of parameters q_j for the construction of new states. Thus, the families of states are sorted by the number of parameters involved. We start with the smallest count of three and then work our way forward to nine parameters where each of the Bell projectors is assigned its own coefficient q_j .

The first two subchapters 6.2.1 and 6.2.2 treat classes of states where, in fact, no bound entanglement could have been found, neither by MUBs nor SICs. But they are still important, not only because they show some interesting features but to give an impression of how the procedure of the search for bound entanglement is performed: First, we will introduce one family of states and explain which entanglement witnesses have been applied to them. Then the witnesses are optimized, meaning that their expectation values are minimized over the parameters $\{q_j\}$ in order to maximize their performance in entanglement detection. Afterwards the results of the MUB-witnesses are analyzed and discussed before moving on to the SICs doing the same. Finally we can make some comparisons about the witnesses' efficiency and utility when it comes to the detection of bound entanglement.

The remaining subchapters (families of states with five or more parameters) are restricted to the outcomes of a selection of optimized witnesses in tabular form and some of those operators will be plotted to give a graphic visualization of discovering (bound) entanglement. The output data in the tables are again analyzed and interpreted for both MUBs and SICs. All of the families of states examined there have turned out to be a success, i.e. bound entanglement detection is possible there, at least when working with MUB-witnesses.

However, it should be noted that while working on this study, more than forty classes of states have been tested and only a few of them have made it to be treated or mentioned here. Their output of entanglement was just too small and/or bound entanglement was not found at all.

Before attending to the parameter-dependent states we have to take into account some relations between important entanglement witnesses that have been ascertained while working on this thesis. Since they were quite often exploited in search of bound entanglement, in particular for saving time, they should be listed here.

The following identities and non-identities of MUB-witnesses, as defined in eq.(4.16), hold (at least) in bipartite qutrit systems, independent of the specific state ("+" = "and", e.g., W_{01} on $(B_1 + B_2)$ means that the Weyl operator W_{01} is applied to both MUBs B_1 and B_2 , while "/" = "either-or"):

- $W_{01} \text{ on } B_1 = W_{01} \text{ on } (B_1 + B_2) = W_{01} \text{ on } B_1 + W_{02} \text{ on } B_2$
- $W_{02} \text{ on } B_1 = W_{02} \text{ on } (B_1 + B_2) = W_{02} \text{ on } B_1 + W_{01} \text{ on } B_2$
- $W_{01} / W_{02} \text{ on } B_2 = W_{00} = \mathbb{1}$
- $W_{01} / W_{02} \text{ on } B_3 \neq W_{01} / W_{02} \text{ on } B_4 \neq W_{01} / W_{02} \text{ on } B_1 \neq W_{00}$
- $W_{01} / W_{02} \text{ on } (B_1 + B_2 + B_3) \neq W_{01} / W_{02} \text{ on all MUBs } (\{B_j\}_{j=1}^4)$
- $W_{01} \text{ on } B_1 = W_{11} \text{ on } B_1 = W_{21} \text{ on } B_1$
- $W_{02} \text{ on } B_1 = W_{12} \text{ on } B_1 = W_{22} \text{ on } B_1$
- $W_{10} \text{ on } B_1 = W_{20} \text{ on } B_1 \neq W_{01} / W_{02} \text{ on } B_1$
- $W_{12} \text{ on } B_2 = W_{21} \text{ on } B_2 = W_{22} \text{ on } B_2 \neq W_{11} \text{ on } B_2 \neq W_{01} / W_{02} \text{ on } B_1$
- $W_{12} \text{ on } B_2 + W_{21} \text{ on } B_3 \neq W_{21} \text{ on } B_2 + W_{12} \text{ on } B_3$,

where B_j represents the j^{th} MUB, arranged in (4.9), and W_{kl} marks the Weyl operators, shown in (2.14), that are used to interchange the MUB-vectors in Bob's subsystem for the construction of entanglement witnesses. The Weyl matrices are only applied to the above-mentioned MUBs, the rest of the basis vectors is not affected at all, i.e. not reordered.

Unfortunately, no identities have been found for the SIC-witnesses. This is mainly because most of them have quite different upper bounds for separable states and thus they needed to be corrected individually. There are still some witnesses like W_{01} or W_{02} applied to the first or the second or any other of the nine SICs which all yield the same deviation from the SIC-criterion in eq.(5.15), yet such cases are very rare. But even those witnesses do not coincide although they often give the same expectation value when employed on any state. Hence, we can only note some relevant non-identities for the SIC-witnesses, as defined in eq.(5.16) - again independent of the specific family of states they are applied to ("+" = and, "/" = or):

- $W_{01} \text{ on } |s_1\rangle \neq W_{01} \text{ on } |s_n\rangle \text{ (} n \neq 1 \text{)}$
- $W_{02} \text{ on } |s_1\rangle \neq W_{02} \text{ on } |s_n\rangle \text{ (} n \neq 1 \text{)}$
- $W_{01} \text{ on } |s_1\rangle + W_{02} \text{ on } |s_2\rangle \neq W_{02} \text{ on } |s_1\rangle + W_{01} \text{ on } |s_2\rangle$
- $W_{01} \text{ on } (|s_1\rangle + |s_2\rangle) \neq W_{01} \text{ on } |s_1\rangle$

- W_{02} on $(|s_1\rangle + |s_2\rangle) \neq W_{02}$ on $|s_1\rangle$
- W_{01} on $(|s_1\rangle + |s_4\rangle) \neq W_{01}$ on $(|s_1\rangle + |s_7\rangle)$
- W_{02} on $(|s_1\rangle + |s_4\rangle) \neq W_{02}$ on $(|s_1\rangle + |s_7\rangle)$
- W_{01} on $(|s_1\rangle + |s_4\rangle / |s_7\rangle) \neq W_{02}$ on $(|s_1\rangle + |s_4\rangle / |s_7\rangle)$
- W_{02} on $|s_1\rangle + W_{01}$ on $|s_4\rangle \neq W_{01}$ on $|s_1\rangle + W_{02}$ on $|s_7\rangle \neq W_{02}$ on $|s_4\rangle + W_{01}$ on $|s_7\rangle$
- W_{01} on $(|s_1\rangle + |s_4\rangle + |s_7\rangle) \neq W_{02}$ on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$,

where $n = \{1, \dots, 9\}$ enumerates the d^2 SIC-POVM elements $|s_n\rangle$, listed in (5.11). Adding a phase to the Weyl operators, i.e. W_{kl} with $k \neq 0$, is useless because the upper bounds of the witnesses then start to vary even stronger, which results in entanglement operators more different to each other.

6.2.1 Three Parameters

We start with the simplest class of states characterized by only three parameters. At first, it was intended to use at least four parameters in order to weight the Bell projectors sufficiently different, as it has been done in Ref. [12]. This should generate heavily mixed states such that finding bound entanglement is more likely. However, as we will see this has proved to be less successful than it was initially expected which is why the number of parameters was varied then. Before taking the next step and increasing the count of coefficients q_j , it was thought that the case of just three parameters should be investigated, for the sake of completeness, as well. The following family of states embedded in the magic simplex has been studied:

$$\rho_{3q} = \left(1 - \sum_{j=1}^{d=3} q_j\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \sum_{j=1}^d \sum_{i=0}^{d-1} \frac{q_j}{d} P_{ij-1}. \quad (6.7)$$

Since several other three-parametric states have yielded identical or very similar results to this one, we will only present ρ_{3q} in this subsection. For clarity and comparison purposes, we need a proper enumeration of the different families of states. That is why all of the states we will address and analyze in this work, are marked by the number of parameters q_j used, and, if more than one state is considered with the same number of q_j 's, another index to enumerate them such as for example $\rho_{1,3q}$.

As one can see in figure 6.2.1, the parameters cover the Bell projectors (see eq.(6.2)) in three parallel vertical columns in this state:



Figure 6.2.1: Graphical representation of the Bell projectors $\{P_{kl}\}_{k,l=0}^{d-1}$ distributed among parameters $\{q_j\}_{j=1}^3$ setting up state ρ_{3q} in the magic simplex (see also figure 6.1.1).

The two MUB-witnesses showing the best outcomes which have been found for state ρ_{3q} are constructed via the Weyl operators W_{01} and W_{02} applied to B_1 , respectively. If those witnesses, noted $\mathcal{W}_{M1}$ and $\mathcal{W}_{M2}$, are used on ρ_{3q} , we receive the expectation values (see definition in (4.17))

$$\langle \mathcal{W}_{M1} \rangle_{\rho_{3q}} = \text{Tr}(\rho_{3q} \mathcal{W}_{M1}) = \frac{1}{3}(2 + q_1 + q_2 - 2q_3) \quad (6.8)$$

$$\langle \mathcal{W}_{M2} \rangle_{\rho_{3q}} = \text{Tr}(\rho_{3q} \mathcal{W}_{M2}) = \frac{1}{3}(2 + q_1 - 2q_2 + q_3). \quad (6.9)$$

Minimizing the expectation values over the parameters $\{q_j\}_{j=1}^3$ while keeping the properties of positivity, $\rho \geq 0$, and PPT, $\rho^\Gamma \geq 0$, as defined in (4.18), reveals non-negative results for

$2 - I_{d+1}$ in both cases:

$$\begin{aligned} \langle \mathcal{W}_{M1, opt} \rangle_{\rho_{3q}} &= \min_{q_j} \{2 - I_{d+1}(\rho_{3q}(q_j)) | \rho_{3q}(q_j) \geq 0, \rho_{3q}^\Gamma(q_j) \geq 0\} \\ &= \langle \mathcal{W}_{M2, opt} \rangle_{\rho_{3q}} = 10^{-13} \approx 0. \end{aligned} \quad (6.10)$$

Hence, even optimal MUB-witnesses for this class of states are not able to detect any bound entanglement.

This can be seen by plotting the optimal witnesses: Their two-dimensional graphical outputs for a cut through the magic simplex for ρ_{3q} is shown in figure 6.2.2. Both of the obviously mirrored MUB-witnesses almost cut the PPT-region (which is identical to the region of positivity here and thus overlapping it) but, in fact, they only touch its corners.

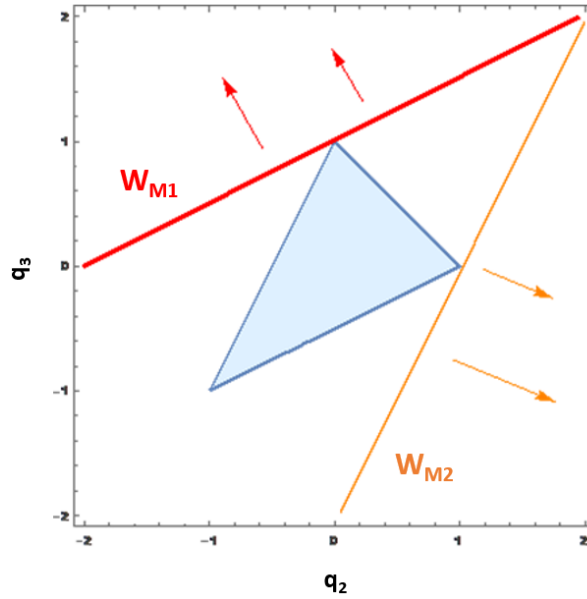


Figure 6.2.2: Cut through the magic simplex where the optimized MUB-witnesses $\mathcal{W}_{M1}$ and $\mathcal{W}_{M2}$ are applied to ρ_{3q} plotted for q_2 and q_3 while $q_1 = 0$ is fixed. The arrows indicate here (and in all following plots), which part of the state space is covered, i.e. detected, by the entanglement witnesses. While $\mathcal{W}_{M1}$ is generated by a cyclic shift via the Weyl operator W_{01} on the first MUB B_1 , $\mathcal{W}_{M2}$ is created analogously by means of W_{02} employed on B_1 . This state and its partially transposed counterpart yield identical eigenvalues, thus the regions of positivity and PPT coincide here (blue triangle).

The outcomes of SIC-witnesses are worse. If we apply again the Weyl operators W_{01} and W_{02} to the first operator, respectively, as we have done with MUBs, i.e. $|s_1\rangle$, we attain for these SIC-witnesses, noted $\mathcal{W}_{S1}$ and $\mathcal{W}_{S2}$, the following expectation values:

$$\langle \mathcal{W}_{S1} \rangle_{\rho_{3q}} = \text{Tr}(\rho_{3q} \mathcal{W}_{S1}) = \frac{1}{24}(21 - 10q_1 + 6q_2 + 4q_3) \quad (6.11)$$

$$\langle \mathcal{W}_{S2} \rangle_{\rho_{3q}} = \text{Tr}(\rho_{3q} \mathcal{W}_{S2}) = \frac{1}{24}(21 - 10q_1 + 4q_2 + 6q_3). \quad (6.12)$$

One has to keep in mind what has been explained in section 5.3. The condition (5.17) has to be checked and, if necessary, modified for each SIC-witness individually in order to obtain a genuine witness. Hence, minimizing the expectation values for $\mathcal{W}_{S1}$ and $\mathcal{W}_{S2}$ means that

$$\langle \mathcal{W}_{opt} \rangle = \min_{q_j} \left\{ \frac{15}{8} - I_{d^2}(\rho(q_j)) | \rho(q_j) \geq 0, \rho^\Gamma(q_j) \geq 0 \right\} \quad (6.13)$$

has to be satisfied. However, the numerical output for the "optimal" expectation values gives

$$\langle \mathcal{W}_{S1, opt} \rangle_{\rho_{3q}} = \langle \mathcal{W}_{S2, opt} \rangle_{\rho_{3q}} = 0.45833, \quad (6.14)$$

which is a distinctly positive result. This is far away from detecting any bound entanglement, these witnesses do not even come close to the area of PPT (and positivity), as one can clearly see in figure 6.2.3.

The best suited SIC-witness that has been found, is constituted by the combination W_{02} on $|s_1\rangle$ and W_{01} on the fourth SIC-vector $|s_4\rangle$. This witness, noted $\mathcal{W}_{S3}$, is illustrated in figure 6.2.4 and is significantly more efficient than $\mathcal{W}_{S1}$ or $\mathcal{W}_{S2}$ but still worse than $\mathcal{W}_{M1}$ and $\mathcal{W}_{M2}$. Computing the expectation value of $\mathcal{W}_{S3}$ applied to state ρ_{3q} gives

$$\langle \mathcal{W}_{S3, opt} \rangle_{\rho_{3q}} = 0.16667. \quad (6.15)$$

$\mathcal{W}_{S3}$ is one of the very few entanglement witnesses which does not need a correction concerning its upper bound on the set of separable states, unlike $\mathcal{W}_{S1}$ and $\mathcal{W}_{S2}$, that is eq.(5.17) is true for $\mathcal{W}_{S3}$ and also for the following witness $\mathcal{W}_{S4}$.

The combination, $\mathcal{W}_{S4} = W_{01}$ (or W_{02}) on $|s_1\rangle$, $|s_4\rangle$ and $|s_7\rangle$ which has turned out to be the second best SIC-witness obtained, yields

$$\langle \mathcal{W}_{S4, opt} \rangle_{\rho_{3q}} = 0.25. \quad (6.16)$$

All other SIC-witnesses, especially those that include roots of unities, i.e. phase shifts - either in the Weyl operator or in the used SIC-vectors (or both) - have provided worse or far worse outcomes, even compared to $\mathcal{W}_{S1}$ or $\mathcal{W}_{S2}$.

Apparently, this easy state is just too symmetric to convey any bound entanglement; at least the methods used here are not able to reveal any PPT-entanglement at all. The regions of positivity and PPT of ρ_{3q} even coincide which is quite often an indicator for a "too balanced" state meaning there is only a little chance of finding bound entanglement. Other possibilities to distribute the three parameters among the Bell states have been tried out as well but all of them have yielded very similar results, in particular without any bound entanglement.

However, ρ_{3q} represents a good example where MUBs clearly provide better results than SICs. Although the MUB-witnesses are not capable of finding any bound entanglement themselves, the differences concerning efficiency are obvious comparing the plots of MUB- and SIC-witnesses to each other. Indeed, we will often experience that shifting MUB-vectors (via Weyl operators) seem to generate better witnesses capable of finding more entanglement than shifted SIC-vectors can do.

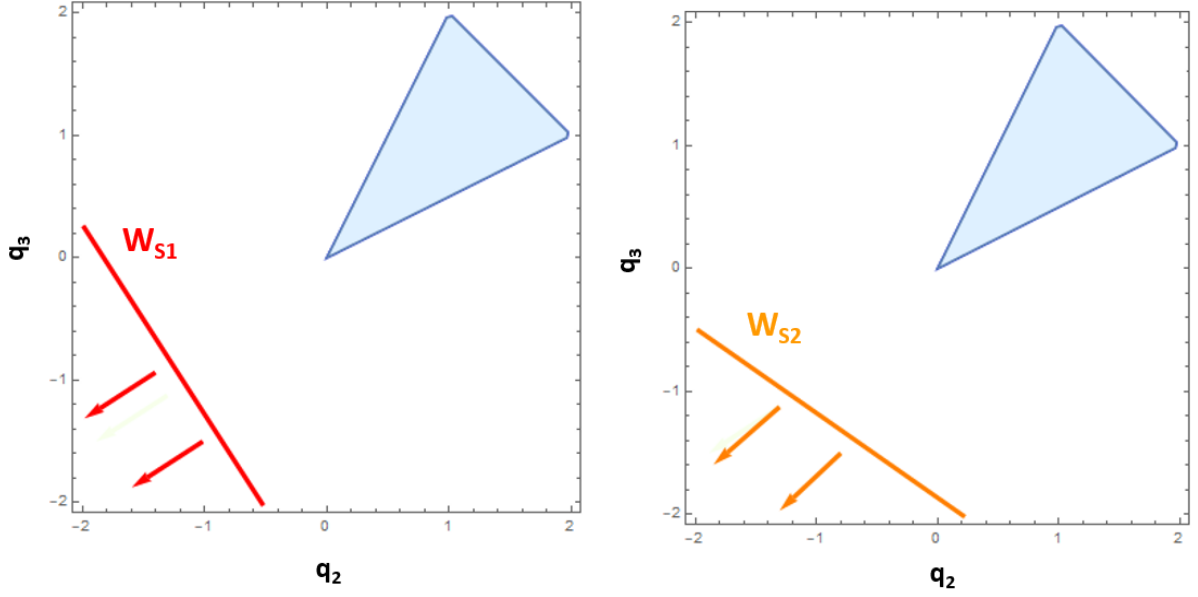


Figure 6.2.3: Cut through the magic simplex where the optimized SIC-witnesses $\mathcal{W}_{S1}$ (left) and $\mathcal{W}_{S2}$ (right) are applied to ρ_{3q} plotted for q_2 and q_3 while $q_1 = 1$ is fixed. $\mathcal{W}_{S1}$ is generated via the Weyl operator W_{01} on the first SIC-vector $|s_1\rangle$, analogously $\mathcal{W}_{S2}$ is constructed using the operator W_{02} on $|s_1\rangle$.

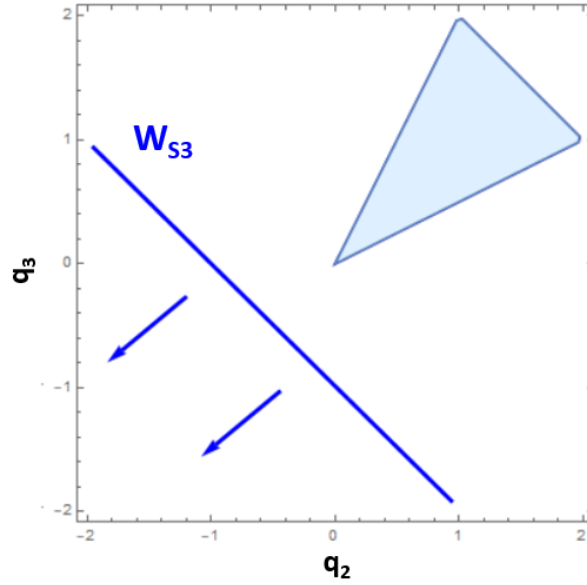


Figure 6.2.4: Optimized SIC-witness W_{02} on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ applied to ρ_{3q} plotted for q_2 and q_3 while $q_1 = 1$ is fixed. The PPT-region, depicted as a blue triangle, is identical to the region of positivity here and overlaps it. This witness covers a significantly larger region than $\mathcal{W}_{S1}$ or $\mathcal{W}_{S2}$, already approaching the zone of PPT (and positivity).

6.2.2 Four Parameters

Now we proceed with families of states containing four parameters. These classes of states have been inspired by the results of a previous master's thesis where (only) MUB-witnesses have been utilized to detect bound entanglement in the magic simplex of one bipartite family of states in different dimensions; see Ref. [45], master's thesis by Eva Kilian: For d dimension $d + 1$ parameters have been employed as coefficients for a various number of Bell states, i.e. in the case of bipartite qutrits the nine Bell projectors have been covered by four parameters. The class of states chosen in Kilian's thesis is based on which has already been explored in Ref. [12]. The construction of the MUB-witnesses there is identical to the way explained here and it has been achieved that two witnesses indeed find some bound entanglement (see also plots in Ref. [45] for graphical illustration, e.g. on page 40).

Since the MUB-witnesses have been successful there, it was just logical to assume the SIC-witnesses might expose some bound entanglement as well. Surprisingly, this has been proven false during the work on this thesis. The SIC-witnesses, as defined in the present work, are not able to detect any form of PPT-entanglement when applied to the qutrit state ($d = 3$) considered in Kilian's thesis, let us call it "Kilian's state" ρ_K :

$$\begin{aligned} \rho_K = & \left(1 - \frac{q_1}{d^2 - (d+1)} - \frac{q_2}{d+1} - q_3 - q_4\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \frac{q_1}{d^2 - (d+1)} P_{00} + \\ & + \frac{q_2}{(d+1)(d-1)} \sum_{i=1}^{d-1} P_{i0} + \frac{q_3}{d} \sum_{i=0}^{d-1} P_{i1} + \frac{q_4}{d} \sum_{i=0}^{d-1} P_{i2}. \end{aligned} \quad (6.17)$$

A graphical illustration of ρ_K in the magic simplex for bipartite qutrits is given in figure 6.2.5. Hence, it was tried to modify this state such that at least some SIC-witnesses (after optimization) are able to detect bound entanglement. A lot of changes have been tested to make this work, at first by keeping just the four parameters. One of them is the interchange of the first two parameter q_1 and q_2 in Kilian's state such that q_1 is now the coefficient for two Bell states (P_{00}, P_{10}) and q_2 just for one (P_{20}). Interestingly, that little modification makes the two effective MUB-witnesses in Ref. [45], which are indeed identical to those applied to state ρ_{3q} in figure 6.2.2, completely useless - even after optimization they are no longer able to detect any bound entanglement at all. Unfortunately, the SIC-witnesses do not improve either. Therefore, an apparently very trivial change in the state can make a big difference about the performance of the witnesses used on it.

Taking ρ_K as initial state, we will now make bigger amendments on it. The next state we consider gives the three Bell projectors in the first phase space line (see first column in the right image in figure 6.2.5) a special treatment:

$$\begin{aligned} \rho_{1,4q} = & \left(1 - \frac{q_1}{d^2 - (d+1)} - \frac{q_2}{d+1} - \frac{q_3}{d-1} - q_4\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \frac{q_1}{d^2 - (d+1)} P_{00} + \\ & + \frac{q_2}{d+1} P_{10} + \frac{q_3}{d-1} P_{20} + \frac{q_4}{2d} \sum_{j=1}^{d-1} \sum_{i=0}^{d-1} P_{ij}. \end{aligned} \quad (6.18)$$

Once more the witnesses $\mathcal{W}_{M1}$ and $\mathcal{W}_{M2}$ constructed by a cyclic shift via the Weyl operators W_{01} or W_{02} on the first MUB B_1 appear to be the best choice when trying to find bound



Figure 6.2.5: Graphical representation of the Bell projectors $\{P_{kl}\}_{k,l=0}^{d-1}$ distributed among parameters $\{q_j\}_{j=1}^4$, separated into different colours, setting up Kilian's state ρ_K (left) and $\rho_{1,4q}$ (right) in the magic simplex.

entanglement. Adding any further shift mostly worsens the efficiency of the witness, even if it is just shifting the vectors within the first two MUBs and in particular, if one adds some phase shifts, i.e. deploying Weyl operators such as W_{10} or W_{21} , in general W_{kl} with $k \neq 0$. The latter also holds for SICs, as we have already ascertained in the analysis of ρ_{3q} .

In this case, the expectation values of $\mathcal{W}_{M1}$ and $\mathcal{W}_{M2}$ are identical:

$$\langle \mathcal{W}_{M1} \rangle_{\rho_{1,4q}} = \langle \mathcal{W}_{M2} \rangle_{\rho_{1,4q}} = \frac{1}{6}(4 - 2q_1 + 2q_2 + 4q_3 - q_4). \quad (6.19)$$

The same minimization procedure we have done in section 6.2.1 is carried out again, now over all four parameters $\{q_j\}_{j=1}^4$. Naturally, this numerical optimization is performed every time we find an appropriate witness since we always want to attain the optimal witness. But the output for the MUB-method is hardly better than we have had with the three-parametric family of states:

$$\begin{aligned} \langle \mathcal{W}_{M1, opt} \rangle_{\rho_{1,4q}} &= \min_{q_j} \{2 - I_{d+1}(\rho_{1,4q}(q_j)) | \rho_{1,4q}(q_j) \geq 0, \rho_{1,4q}^\Gamma(q_j) \geq 0\} = \\ &= 6 \cdot 10^{-9} \approx 0. \end{aligned} \quad (6.20)$$

So this time again, even the optimal MUB-witnesses cannot expose any bound entanglement, which is illustrated in figure 6.2.6. The witness may cut the region of PPT but this is useless because it misses the positivity section.

The expectation values of the SIC-witnesses $\mathcal{W}_{S1}$ and $\mathcal{W}_{S2}$ applied to $\rho_{1,4q}$ yield

$$\langle \mathcal{W}_{S1} \rangle_{\rho_{1,4q}} = \langle \mathcal{W}_{S2} \rangle_{\rho_{1,4q}} = -\frac{7q_1}{20} + \frac{1}{48}(42 + 3q_2 + 6q_3 + 10q_4). \quad (6.21)$$

Optimizing these values (see eq.(6.13)), provides the following solution (for both $\mathcal{W}_{S1}$ and $\mathcal{W}_{S2}$):

$$\langle \mathcal{W}_{S1, opt} \rangle_{\rho_{1,4q}} = 0.43056. \quad (6.22)$$

This is a slightly better result we have had before with the same witnesses on ρ_{3q} but it is again positive and much greater than the corresponding outcome of the optimal MUB-witness $\langle \mathcal{W}_{M1, opt} \rangle_{\rho_{1,4q}}$. However, as before, the witnesses $\mathcal{W}_{S3} = W_{02}$ on $|s_1\rangle + |s_4\rangle$ as well as $\mathcal{W}_{S4} = W_{01}$ on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$ prove again to be the most efficient SIC-witnesses which could have been found:

$$\langle \mathcal{W}_{S3, opt} \rangle_{\rho_{1,4q}} = 0.11111 \quad (6.23)$$

$$\langle \mathcal{W}_{S4, opt} \rangle_{\rho_{1,4q}} = 0.16667. \quad (6.24)$$

Other SIC-witnesses are not worth mentioning because all of them provide worse results than $\mathcal{W}_{S1}$ and thus are even further away from the intersection of PPT and the positivity section. The plots in figure 6.2.6 show the difference in quality between the best MUB- and SIC-witness found, employed on state $\rho_{1,4q}$.

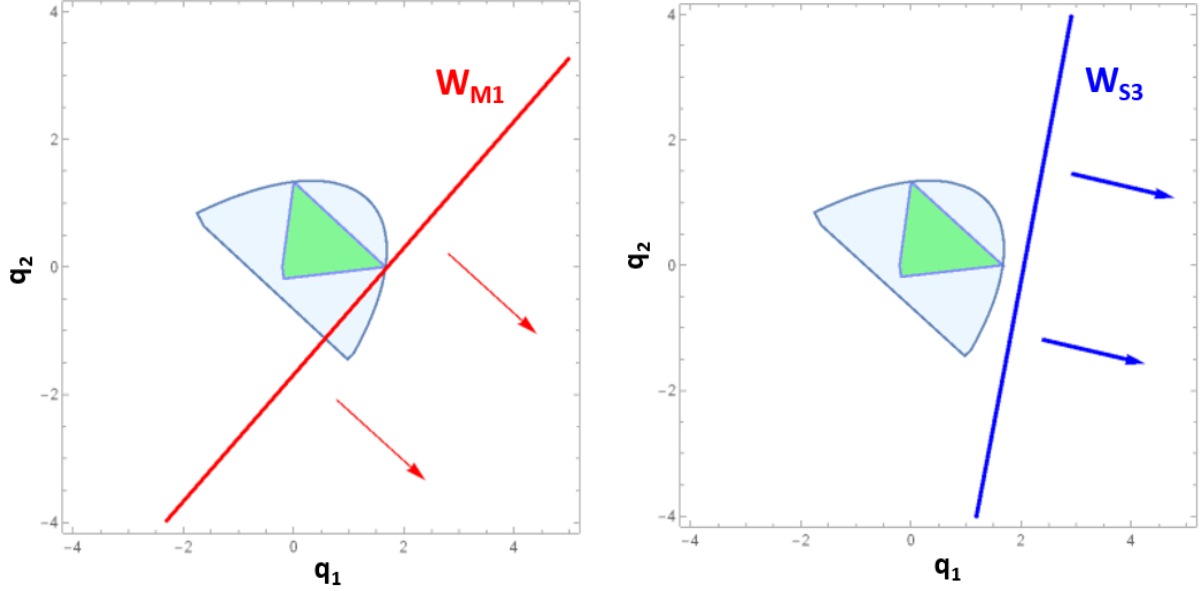


Figure 6.2.6: Optimized MUB-witness $\mathcal{W}_{M1} = W_{01}$ on B_1 (left) and optimized SIC-witness $\mathcal{W}_{S3} = W_{02}$ on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ (right) applied to $\rho_{1,4q}$ plotted for q_1 and q_2 while $q_3 = 0$ and $q_4 = \frac{2}{3}$ are fixed. The green triangle represents the field of positivity while the light blue zone marks the range of PPT which is plotted transparent to a certain degree to show the overlapping areas of positivity and PPT.

State $\rho_{1,4q}$ is a typical example where MUB-witnesses are definitely more efficient in detecting bound entanglement (or actually in approaching it) compared to SIC-witnesses and yet they are not successful either. MUB-witnesses are at least able to touch the wanted area where the conditions of positivity and PPT are satisfied but SIC-witnesses are not even able to do that. Many more families of states have been studied but most of them have yielded very similar results and not any improvements. Hence, $\rho_{1,4q}$ has been analyzed and explained above to represent all of those "failed" states where bound entanglement could not have been found at all using the methods of MUBs or SICs.

Now let us discuss another state that has surprisingly given significantly better outcomes for the optimized SIC-witnesses than all the other treated states with four parameters:

$$\begin{aligned} \rho_{2,4q} = & \left(1 - \frac{q_1}{d^2 - (d+1)} - \frac{q_2}{d+1} - q_3 - q_4\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \frac{q_1}{d^2 - (d+1)} P_{00} + \\ & + \frac{q_2}{(d+1)(d-1)} \sum_{i=1}^{d-1} P_{0i} + \frac{q_3}{d} \sum_{i=0}^{d-1} P_{1i} + \frac{q_4}{d} \sum_{i=0}^{d-1} P_{2i}. \end{aligned} \quad (6.25)$$

In figure 6.2.7 a graphic representation of state $\rho_{2,4q}$ embedded in the magic simplex is shown.



Figure 6.2.7: Graphical representation of the Bell projectors $\{P_{kl}\}_{k,l=0}^{d-1}$ distributed among parameters $\{q_j\}_{j=1}^4$ setting up state $\rho_{2,4q}$ in the magic simplex.

This time we look at the horizontal phase space lines, i.e. the parameters cover the Bell projectors in rows (see figure 6.1.1)) instead of columns as we have done it in ρ_K . As a matter of fact there was no witness found, neither by MUBs nor by SICs, that was able to detect some bound entanglement when applied to $\rho_{2,4q}$. And still it is worth taking a look at this state due to the results it has supplied, in particular if one compares those to the outputs of the witnesses applied to Kilian's state ρ_K .

In table 6.2.1 a selection of optimized MUB- and SIC-witnesses is listed, i.e. their expectation values are (numerically) minimized over all four parameters while maintaining the conditions of positivity and PPT. Those values are then compared between $\rho_{2,4q}$ and ρ_K . The witnesses are chosen such that they generally provide the best outputs which could have been found within the scope of this thesis. Hence, they are not selected randomly although some of them, especially witnesses that include a phase shift, i.e. W_{kl} with $k \neq 0$, could have been replaced by some alternatives but none of them has yielded better outcomes - equally good ones at best. As we have already treated the identities of MUB- and SIC-witnesses in section 6.2, "+" marks a combination while "/" denotes "either-or".

The first column in table 6.2.1 lists the optimized witnesses that are constructed by deploying Weyl shifts W_{kl} on the MUB vectors in eq.(4.16) or on the SIC-vectors in eq.(5.16). The upper part of the table treats the MUB-witnesses while the lower part deals with the SIC-witnesses, both sections separated by a horizontal double line. If these witnesses are applied to Kilian's state ρ_K and $\rho_{2,4q}$, respectively, one obtains the minimized expectation values listed in the second column for ρ_K and in the third column for $\rho_{2,4q}$.

Note that the Weyl shifts W_{01} or W_{02} operating on any other SIC-vector than the first one yields the identical expectation value (even though the witnesses are different).

Optimized witnesses $\mathcal{W}_{opt}$	$\langle \mathcal{W}_{opt} \rangle_{\rho_K}$	$\langle \mathcal{W}_{opt} \rangle_{\rho_{2,4q}}$
W_{01} / W_{02} on B_1	-0.1547	0
W_{01} / W_{02} on B_3	0	0
W_{01} / W_{02} on B_4	0	0
W_{01} on $(B_2 + B_3) + W_{02}$ on $(B_1 + B_4)$	0	0
W_{12} on $B_1 + W_{21}$ on $B_2 + W_{11}$ on $B_3 + W_{22}$ on B_4	0	0
W_{01} / W_{02} on $ s_1\rangle$	0.42967	0.375
W_{01} / W_{02} on $(s_1\rangle + s_2\rangle)$	0.51768	0.41073
W_{01} on $ s_1\rangle + W_{02}$ on $ s_2\rangle$	0.55186	0.44075
W_{02} on $ s_1\rangle + W_{11}$ on $ s_2\rangle$	0.52938	0.5016
W_{11} on $ s_1\rangle + W_{01}$ on $ s_2\rangle$	0.81886	0.79524
W_{01} / W_{02} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	0.48195	0.375
W_{02} on $ s_1\rangle + W_{01}$ on $ s_4\rangle /$		
W_{01} on $ s_1\rangle + W_{02}$ on $ s_7\rangle /$		
W_{02} on $ s_4\rangle + W_{01}$ on $ s_7\rangle$	0.11111	0
W_{01} / W_{02} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	0.15537	0

Table 6.2.1: Optimized expectation values calculated for a set of MUB- and SIC-witnesses applied to the states ρ_K and $\rho_{2,4q}$. MUB- and SIC-witnesses are separated by the horizontal double line at the center of the table. Note that witness W_{01} / W_{02} on B_2 always gives W_{00} which is the identity $\mathbb{1}$, detecting nothing at all. All results $\leq |\pm 10^{-7}|$ are rounded to zero.

As we can see in the upper table, even the optimized MUB-witnesses cannot detect any bound entanglement when applied to $\rho_{2,4q}$ - all witnesses supply very small results ($\approx 10^{-8} \sim 0$) but none is negative. In fact, only the witnesses W_{01} or W_{02} on B_1 which we have noted $\mathcal{W}_{M1}$ and $\mathcal{W}_{M2}$ before, used on ρ_K are able to find some PPT-entanglement as already stated previously. But if we move on to the SIC-witnesses, we can determine that all of the results of $\rho_{2,4q}$ have indeed improved in comparison to ρ_K . Most of them are clearly worse than the outputs of any MUB-witness but, still, concerning only the optimized expectation values of all the SIC-witnesses tested on various families of states with different numbers of parameters, these outcomes belong to the best in this entire study.

A visualization of one of the most efficient SIC-witnesses from table 6.2.1, $\mathcal{W}_{S4} = W_{01}$ on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$, operating on both ρ_K and $\rho_{2,4q}$ for comparison purposes, can be seen in figure 6.2.8. The same witness is able to detect more (free) entanglement in state $\rho_{2,4q}$ than in Kilian's state and even touches the tip of the triangular PPT section but in either case it does not register any bound entanglement.

Why does state $\rho_{2,4q}$ give better results for SIC-witnesses than Kilian's state? Comparing the phase space structure of the two states, the only significant difference between them is that the line states are covered horizontally by the parameters q_j in $\rho_{2,4q}$ and vertically in ρ_K . Due to that the MUB-witnesses obviously become worse while the SIC-ones are enhanced. Is this just a coincidence or may there be an underlying subtle (phase space) structure of SIC-POVMs which could explain those discrepancies. Several other classes of states with four or more

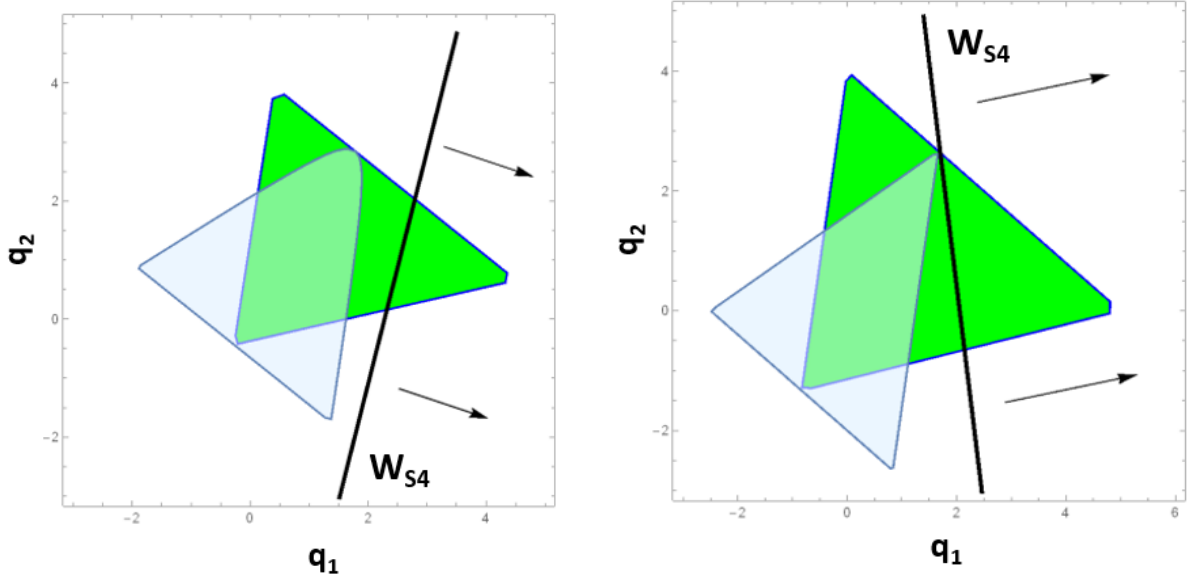


Figure 6.2.8: SIC-witness $\mathcal{W}_{S4} = W_{01}$ on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$ applied to both ρ_K (left) and $\rho_{2,4q}$ (right) plotted for q_1 and q_2 with q_3 and q_4 fixed. The green triangle represents the area of positivity and the blue partially transparent one marks the range of PPT.

parameters have been examined to reproduce this phenomenon that seems to be caused by the opposite usage of the phase space lines (e.g. instead of columns take rows, similar to a transposition). However, it has been impossible to gain another such situation, at least in this significant extent of non-conformance, when working with only four-parametric families of states. Most of the differences in results are very small which can be ascribed to fluctuations. But there have been discovered some states with higher parameterizations that have provided a very similar output for the same SIC-witnesses, as $\rho_{2,4q}$ shows here.

Looking at the results from table 6.2.1, another important question emerges: What about the last two witnesses $\mathcal{W}_{S3} = W_{02}$ on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ (and its equivalent variants as stated above) as well as $\mathcal{W}_{S4} = W_{01} / W_{02}$ on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$? We have already discussed their results in the states ρ_{3q} and $\rho_{1,4q}$ and again they appear as the most successful SIC-witnesses. They yield the smallest minimized expectation values so far, albeit non-negative and thus no bound entanglement. Applied to state $\rho_{2,4q}$, they are even equally efficient as the MUB-witnesses. At first, one could argue again that these numerical differences are caused by the non-inclusion of phase shifts in the creation of the witnesses, either in the Weyl operators such as W_{11} or in the used SIC-vectors, e.g. $|s_2\rangle$, or in both of them. And indeed, if one analyzes the data above, adding any phase shift generally seems to worsen the efficiency of any witness. However, W_{01} / W_{02} on $|s_1\rangle$ or the combinations W_{01} / W_{02} on $(|s_1\rangle + |s_4\rangle / |s_7\rangle)$ do not have any roots of unity, ω , at all and still they provide far worse results than $\mathcal{W}_{S3}$ or $\mathcal{W}_{S4}$ - hardly better than any of the other witnesses.

Hence, the last five witnesses ($\mathcal{W}_{S3}$ and $\mathcal{W}_{S4}$ are representative for them) in table 6.2.1 are obviously somewhat special, which is an observation we will often make: Although there is a

vast amount of possible permutations shifting the order of MUB- and SIC-vectors with Weyl operators, the best results obtainable are mostly attained by utilizing the witnesses $\mathcal{W}_{M1}/\mathcal{W}_{M2} = W_{01}/W_{02}$ on B_1 for the MUB-method and $\mathcal{W}_{S3}$ and $\mathcal{W}_{S4}$ for the SIC-method. Apparently, the remarkable behavior of these two witnesses has to do with another interesting phenomenon: The larger the upper bound of a SIC-witness is, the lower its entanglement detection efficiency, which can be seen in the following table:

SIC-witnesses	Upper Bound	$\langle \mathcal{W}_{opt} \rangle_{\rho_K}$	$\langle \mathcal{W}_{opt} \rangle_{\rho_{2,4q}}$
W_{01} / W_{02} on $ s_1\rangle$	1.875	0.42967	0.375
W_{01} / W_{02} on $(s_1\rangle + s_2\rangle)$	1.91073	0.51768	0.41073
W_{01} on $ s_1\rangle + W_{02}$ on $ s_2\rangle$	1.94075	0.55186	0.44075
W_{02} on $ s_1\rangle + W_{11}$ on $ s_2\rangle$	1.91827	0.52938	0.5016
W_{11} on $ s_1\rangle + W_{01}$ on $ s_2\rangle$	2.21191	0.81886	0.79524
W_{01} / W_{02} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	1.875	0.48195	0.375
W_{02} on $ s_1\rangle + W_{01}$ on $ s_4\rangle /$ W_{01} on $ s_1\rangle + W_{02}$ on $ s_7\rangle /$			
W_{02} on $ s_4\rangle + W_{01}$ on $ s_7\rangle$	1.5	0.11111	0
W_{01} / W_{02} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	1.5	0.15537	0

Table 6.2.2: The upper bound calculated individually for the most relevant SIC-witnesses compared to the optimized expectation values of the same witnesses when applied to the states ρ_K and $\rho_{2,4q}$. Again, results $\leq |\pm 10^{-7}|$ are rounded to zero.

The true, corrected upper bound on separable states of each SIC-witness, as listed in the table above, is independent of any family of states the witness is applied to. Looking at the output data, the witnesses with a smaller upper bound like W_{01} / W_{02} on $|s_1\rangle$ or W_{02} on $|s_4\rangle + W_{01}$ on $|s_7\rangle$ obviously give better, i.e. smaller, (optimized) expectation values for both ρ_K and $\rho_{2,4q}$. This correlation between upper bound and detection performance has also been ascertained when working with any other class of states examined for this thesis. However, comparing the results of ρ_K and $\rho_{2,4q}$ to each other, it is clear that the SIC-witness' efficiency is not (fully) independent of the utilized family of states. As an example, the last witness W_{01} / W_{02} on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$ has the lowest upper bound found of all SIC-witnesses tested and, still, its minimized expectation value for $\rho_{2,4q}$ is significantly smaller than for ρ_K . Such excellent outcomes for SIC-witnesses (even though no bound entanglement could be gained) have only emerged rarely. In fact, just a handful of states have supplied very similar results for the optimized SIC-witnesses as $\rho_{2,4q}$ has. Two of them are presented in the later sections where more parameters are used. Anyway, it is an important and useful observation that for some special witnesses employed on certain classes of states, the capability to detect entanglement exploiting SICs can be greatly boosted.

6.2.3 Five Parameters

Now we will move on and increase the number of parameters continuously in order to attain families of states which are more (heavily) mixed than all the states before. That should enhance the chance to detect bound entanglement and, in fact, it does, as we will see. We start with the introduction of a fifth parameter in this subsection and discuss four bipartite qutrit classes of states rendering quite surprising results.

From now on, the same MUB- and SIC-witnesses presented in table 6.2.1 will be applied to all families of states that are to be analyzed in this thesis. This is done to guarantee a better comparison of all the findings of the states under investigation among MUBs and SICs, respectively, but also between them. Furthermore, looking through the complete output data of this study, that selection of witnesses generally performs the best detection of entanglement. First we present the four five-parametric families of states that are to be discussed here and then we will list all of the outcomes of the main (optimized) entanglement witnesses for both methods in one table in order to improve the lucidity of the survey.

Let us begin with a simple but effective adaption of state $\rho_{1,4q}$ (6.18):

$$\begin{aligned} \rho_{1,5q} = & \left(1 - \frac{q_1}{d^2 - (d+1)} - \frac{q_2}{d+1} - \frac{q_3}{d-1} - q_4 - q_5\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \frac{q_1}{d^2 - (d+1)} P_{00} + \\ & + \frac{q_2}{d+1} P_{10} + \frac{q_3}{d-1} P_{20} + \frac{q_4}{d} \sum_{i=0}^{d-1} P_{i1} + \frac{q_5}{d} \sum_{i=0}^{d-1} P_{i2}. \end{aligned} \quad (6.26)$$

Based on $\rho_{1,4q}$, the Bell projectors P_{kl} making up the second and third vertical phase space line, are now weighted individually by the parameters q_4 and q_5 while the first line is again divided into three parameters, one for each P_{kl} (for graphical illustration see figure 6.2.9).

The next class of state is generated by modifying Kilian's state ρ_K in the second line state covered by q_3 . It is now split into a combination of P_{kl} unequally distributed among two parameters - its depiction in the magic simplex for bipartite qutrits is shown in figure 6.2.9, right-sided:

$$\begin{aligned} \rho_{2,5q} = & \left(1 - \frac{q_1}{d^2 - (d+1)} - \frac{q_2}{d+1} - \frac{q_3}{d+1} - \frac{q_4}{d^2 - (d+1)} - q_5\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \\ & + \frac{q_1}{d^2 - (d+1)} P_{00} + \frac{q_2}{(d+1)(d-1)} \sum_{i=1}^{d-1} P_{i0} + \frac{q_3}{(d+1)(d-1)} \sum_{i=0}^{d-2} P_{i1} + \\ & + \frac{q_4}{d^2 - (d+1)} P_{21} + \frac{q_5}{d} \sum_{i=0}^{d-1} P_{i2}. \end{aligned} \quad (6.27)$$

It should be noted here that dimensional coefficients such as $\frac{1}{d^2 - (d+1)}$ or $\frac{1}{d+1}$ in the unity of the upper state do not affect the (optimized) expectation values of the witnesses and thus their entanglement detection efficiency. In fact, they are mainly used to facilitate the calculation of the eigenvalues of the parametric state and the eigenvalues of its partial transposition. But sometimes, as in the following two cases, those coefficients do not help at all or make



Figure 6.2.9: Graphical representation of the $\{P_{kl}\}_{k,l=0}^{d-1}$ distributed among parameters $\{q_j\}_{j=1}^5$ forming the states $\rho_{1,5q}$ (left) and $\rho_{2,5q}$ (right) in the magic simplex.

computations easier, that is why they are left out then.

Now we perform a little change on the previous state $\rho_{2,5q}$ concerning parameters q_3 and q_4 :

$$\begin{aligned} \rho_{3,5q} = & \left(1 - \sum_{j=1}^5 q_j\right) \frac{1}{d^2} \mathbb{1}_{d^2} + q_1 P_{00} + \frac{q_2}{d-1} \sum_{i=1}^{d-1} P_{i0} + q_3 P_{11} + \frac{q_4}{d-1} (P_{01} + P_{21}) + \\ & + \frac{q_5}{d} \sum_{i=0}^{d-1} P_{i2}. \end{aligned} \quad (6.28)$$

The last of the families of states characterized by five parameters is quite different to those considered so far. It can be seen as a special experiment which has shown very remarkable results:

$$\begin{aligned} \rho_{4,5q} = & \left(1 - \sum_{j=1}^5 q_j\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \frac{q_1}{d-1} \sum_{i=0}^{d-2} P_{i0} + q_2 P_{01} + \frac{q_3}{d} (P_{20} + P_{11} + P_{02}) + \\ & + q_4 P_{12} + \frac{q_5}{d-1} \sum_{i=1}^{d-1} P_{2i}. \end{aligned} \quad (6.29)$$

To get a graphic idea of how the projectors weighted by the parameters form this state (and also $\rho_{3,5q}$) in the magic simplex, have a look at figure 6.2.10.

These classes of states all have been successful generating bound entanglement witnesses, except for the last one, $\rho_{4,5q}$. But this state shows some properties in its outcomes which makes it unique justifying its consideration here. The following table gives the data on the most efficient witnesses that could have been found. Their expectation values for the states presented above are optimized to receive the maximally possible amount of bound entanglement. The table is structured the same way as table 6.2.1 and thus the applications of "+" for more than one Weyl operator and "/" for either this operator or another one generating identical results, are used again. This time the optimized expectation values such as $\langle \mathcal{W}_{opt} \rangle_{\rho_{1,5q}}$ are abbreviated solely as $\rho_{1,5q}$.



Figure 6.2.10: Bell projectors $\{P_{kl}\}_{k,l=0}^{d-1}$ distributed among parameters $\{q_j\}_{j=1}^5$ creating the states $\rho_{3,5q}$ (left) and $\rho_{4,5q}$ (right) in the magic simplex.

Optimized witnesses $\mathcal{W}_{opt}$	$\rho_{1,5q}$	$\rho_{2,5q}$	$\rho_{3,5q}$	$\rho_{4,5q}$
W_{01} / W_{02} on B_1	-0.1547	-0.1547	-0.1547	0.40457
W_{01} on B_3	0	-0.01342	0	0.19098
W_{02} on B_3	0	0	0	0.2
W_{01} on B_4	0	0	-0.01342	0
W_{02} on B_4	0	0	0	0.0623
W_{01} on $(B_2 + B_3) +$ $+ W_{02}$ on $(B_1 + B_4)$	0	0	0	0.10539
W_{12} on $B_1 + W_{21}$ on $B_2 +$ $+ W_{11}$ on $B_3 + W_{22}$ on B_4	0	0	0	0
W_{01} on $ s_1\rangle$	0.42967	0.42967	0.42967	0.56067
W_{02} on $ s_1\rangle$	0.42967	0.42884	0.42884	0.5652
W_{01} on $(s_1\rangle + s_2\rangle)$	0.51768	0.51768	0.51768	0.63328
W_{02} on $(s_1\rangle + s_2\rangle)$	0.51768	0.51413	0.51413	0.62914
W_{01} on $ s_1\rangle + W_{02}$ on $ s_2\rangle$	0.55186	0.55082	0.55082	0.67495
W_{02} on $ s_1\rangle + W_{11}$ on $ s_2\rangle$	0.52938	0.52834	0.52834	0.66006
W_{11} on $ s_1\rangle + W_{01}$ on $ s_2\rangle$	0.81886	0.81886	0.81886	0.95311
W_{01} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	0.48195	0.48195	0.48195	0.59755
W_{02} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	0.48195	0.4784	0.4784	0.5934
W_{02} on $ s_1\rangle + W_{01}$ on $ s_4\rangle /$ W_{01} on $ s_1\rangle + W_{02}$ on $ s_7\rangle /$				
W_{02} on $ s_4\rangle + W_{01}$ on $ s_7\rangle$	0.11111	0.11007	0.11007	0.2342
W_{01} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	0.15537	0.15537	0.15537	0.25
W_{02} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	0.15537	0.14694	0.14694	0.22805

Table 6.2.3: Minimized expectation values over all five parameters calculated for a set of MUB- and SIC-witnesses applied to the states $\rho_{1,5q}$, $\rho_{2,5q}$, $\rho_{3,5q}$ and $\rho_{4,5q}$. MUB- and SIC-witnesses are separated by the horizontal double line at the center of the table. All results $\leq |\pm 10^{-7}|$ are rounded to zero.

According to table 6.2.3, the MUB-witnesses generated by the Weyl-shifts W_{01} or W_{02} used on the vectors of the first MUB seem to be again the most efficient operators for entanglement detection. For states $\rho_{1,5q}$, $\rho_{2,5q}$ and $\rho_{3,5q}$ these two witnesses expose a significant

amount of bound entanglement. Interestingly, it is just as much as the optimal value for bound entanglement Kilian's state ρ_K for the same witnesses has provided. Is it possible that $-0.1547 = 1 - \frac{2}{\sqrt{3}}$ is the maximal volume of bound entanglement any (optimized) MUB-witness can detect, at least in bipartite qutrit systems?

If we just look at the outcomes of the other MUB-witnesses applied to the first three five-parametric states, we can see that none of them is capable of finding some bound entanglement, even in the optimal case - with two exceptions: One of them is established by employing W_{01} on the third mutually unbiased base in state $\rho_{2,5q}$ and the other one by the same Weyl operator on the fourth MUB in $\rho_{3,5q}$. Both of them yield -0.01342 as a result, hence they are indeed the first witnesses apart from W_{01} / W_{02} on B_1 which can discover bound entanglement although their detection range is far smaller. The minimized expectation values of W_{01} / W_{02} on the first MUB used on $\rho_{1,5q}$, $\rho_{2,5q}$ or $\rho_{3,5q}$ are in fact more than eleven times smaller compared to the values of these two witnesses, thus the size of the bound entanglement area they can reveal is eleven times larger.

Graphical plots in figure 6.2.11 show this huge difference in an exemplary way for state $\rho_{2,5q}$: $\mathcal{W}_{M1}$ is the short notation for the witness W_{01} on B_1 and $\mathcal{W}_{M3}$ for W_{01} on B_3 . While the field of detected bound entanglement is very well recognizable for (optimized) $\mathcal{W}_{M1}$, it can hardly be seen for (optimized) $\mathcal{W}_{M3}$. Naturally, one could have also taken the corresponding witnesses for $\rho_{3,5q}$ for this comparison but their graphic representations are not that expressive.

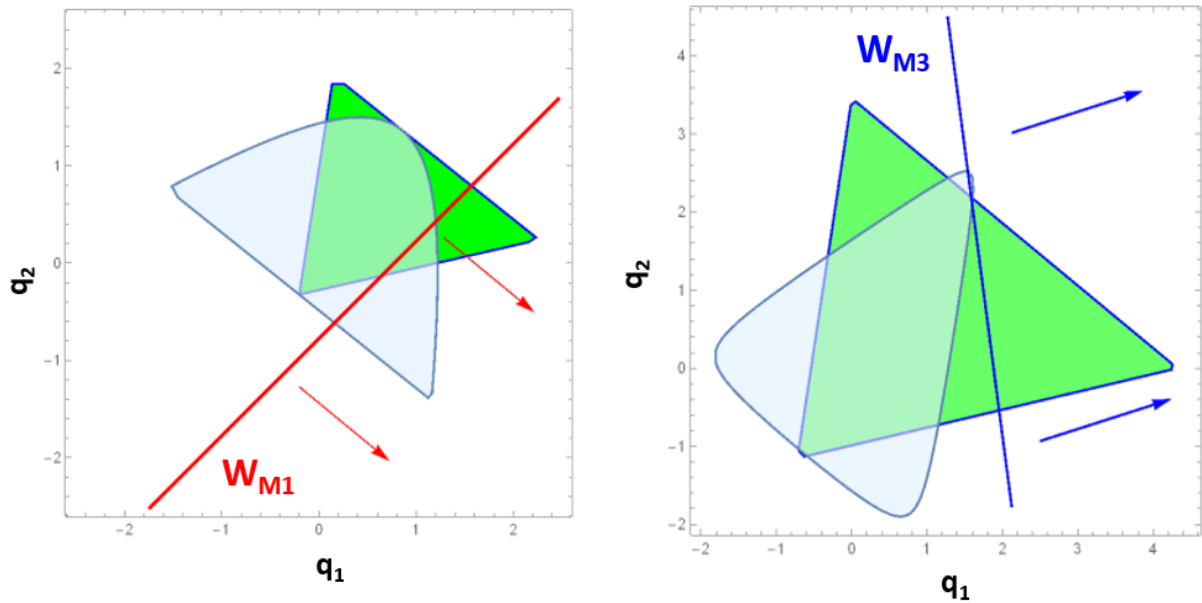


Figure 6.2.11: MUB-witnesses $\mathcal{W}_{M1} = W_{01}$ on B_1 (left) and $\mathcal{W}_{M3} = W_{01}$ on B_3 (right) applied to $\rho_{2,5q}$ plotted for q_1 and q_2 while the remaining parameters q_3 , q_4 and q_5 are fixed. The green triangle represents the region of positivity and the light blue transparent field marks the region of PPT. The small area with overlapped positivity and PPT, exposed by the witness, displays the zone of bound entanglement.

Changing the order of vectors within MUBs other than the first one by implementing local

shifts does generally not yield any bound entanglement, which has been tested in many more families of states than those listed in table 6.2.3. But sometimes there are exceptions like W_{01} on B_3 in $\rho_{2,5q}$ or W_{01} on B_4 in $\rho_{3,5q}$ that probably give the same negative expectation value here due to the similarities of the structures of the states - only q_3 and q_4 are differently preferred. However, the main question is what this -0.01342 actually means.

When computing the minimized expectation value for diverse MUB-witnesses the output was often very small, varying from $\pm(10^{-7}$ to $10^{-9})$, rounded to zero as an official result. Is the value -0.01342 , at least five orders of magnitude larger, just a very strong fluctuation around zero that only occurs for some special witnesses? As we can see, the very same value emerges for two different states for distinct witnesses and there have been some further states not mentioned here yielding the identical result. In addition, other states characterized by more than five parameters, as we will see in the next subsection, have also supplied negative outcomes with only some hundredths below zero for various MUB-witnesses. Therefore, the findings do not suggest a fluctuation, not just a coincidence. These witnesses do detect a certain amount of bound entanglement and thereby are more successful than others, even though they are by far not as suitable as those constructed from the Weyl-operators W_{01}/W_{02} used on B_1 .

What about the output data of state $\rho_{4,5q}$? Even optimizing the MUB-witnesses employed on this state does not render any PPT-entanglement at all. However, the results do improve if one replaces the best witnesses so far, $\mathcal{W}_{M1} = W_{01}$ on B_1 and $\mathcal{W}_{M2} = W_{02}$ on B_1 , by a different one, such as W_{01} on B_4 or a combination of different Weyl operators applied to various mutually unbiased bases like the last MUB-witness listed in table 6.2.3. It is a very surprising fact that $\mathcal{W}_{M1}$ and $\mathcal{W}_{M2}$ appear as two of the worst witnesses for $\rho_{4,5q}$. In particular, including roots of unity, i.e. deploying Weyl operators such as W_{11} or W_{21} , in general W_{kl} with $k \neq 0$, does not worsen the efficiency of the witness, as it has done so far. On the contrary, concerning this specific state, phase shifts often seem to enhance it although expectation values below zero have never been reached.

The reason for this extraordinary behavior is presumably the distinct manner in which the parameters cover the nine Bell projectors: q_3 treats a diagonal phase space line and, in addition, two further parameters q_1 and q_5 cover partly a vertical and a horizontal phase space line. There have been analyzed a lot of other states quite similar to $\rho_{4,5q}$, many of them including a diagonal phase space line as well but only a few of them could reproduce comparable outcomes showing properties like those of $\rho_{4,5q}$. In such cases the usually reliable witnesses $\mathcal{W}_{M1} / \mathcal{W}_{M2}$ have mostly turned out to be very bad witnesses while all the others have provided (at least slightly) better results. It is the exact opposite performance of the same witnesses applied to $\rho_{1,5q}$, $\rho_{2,5q}$ and $\rho_{3,5q}$ and almost all the other states tested for this thesis. Also, this behavior of the entanglement witnesses demonstrates the dependence on the given class of states. Since all Bell states P_{kl} (see eq.(6.2) and eq.(2.13)) need to be involved to synthesize the families of states in the magic simplex, Weyl operators W_{kl} with $k \neq 0$ and thus phases are naturally contained within state construction. In this sense, local shifts and phase shifts are both essential for the efficacy of the witnesses and can enhance or worsen them, showing distinctive state-dependence.

Nonetheless, $\rho_{4,5q}$ and states of a similar structure cannot detect any bound entanglement that is why any graphic visualization would be pointless here. But they clearly show that there are some exceptions regarding the apparent rule that the MUB-witness generated by $W_{01} /$

W_{02} on B_1 used on an arbitrary state always has to bring the best detection efficiency, i.e. the smallest expectation values. Other witnesses can sometimes do better, so, one should not rely on the simplest Weyl shifts operating solely on the first MUB. However, the occurrence of such special states like $\rho_{4,5q}$ has been quite rare (within the scope of this study) and, in fact, they have only been found by accident.

The findings of the witnesses constructed by SIC-POVMs are again anything but satisfactory. The minimized expectation values of all of them are much greater than zero, meaning that even the optimized SIC-witnesses do not come close to the target area at all where the necessary ingredients for bound entanglement are united: positivity, PPT and entanglement as it is illustrated for MUB-witness $\mathcal{W}_{M1}$ in the left graphic in figure 6.2.11.

State $\rho_{4,5q}$ cannot afford surprises as we have had with MUBs before. All SIC-witnesses, not only those noted in table 6.2.3, tested out for this state but also for the others, $\rho_{1,5q}$, $\rho_{2,5q}$ and $\rho_{3,5q}$, exhibit the same pattern we have already recognized in table 6.2.1: Adding Weyl operators like W_{11} , containing roots of unity, always increases the expectation values significantly, diminishing the chance of detecting bound entanglement even further. But witnesses exploiting only W_{01} or W_{02} and the SIC-vectors $|s_1\rangle$, $|s_4\rangle$ and $|s_7\rangle$ generally reduce the expectation value, where W_{02} on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ (and the two witnesses yielding identical outcomes) and W_{01} or W_{02} on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$ turn out to be again the most efficient SIC-witnesses. The reasons for this phenomenon have already been discussed in section 6.2.2. Interestingly, using W_{02} gives sometimes a slightly better output than W_{01} , like, e.g., in W_{01}/W_{02} on $(|s_1\rangle + |s_4\rangle / |s_7\rangle)$ or the last witness in table 6.2.3, W_{01}/W_{02} on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$.

In figure 6.2.12, the difference in quality, i.e. entanglement detection efficiency, between the first and simplest SIC-witness, W_{01} on $|s_1\rangle$, noted $\mathcal{W}_{S1}$, the best one, $\mathcal{W}_{S3} = W_{02}$ on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ and the worst among all SIC-witnesses stated in table 6.2.3, $\mathcal{W}_{S5} = W_{11}$ on $|s_1\rangle + W_{01}$ on $|s_2\rangle$ is plotted for $\rho_{2,5q}$. All three of them are capable of finding entanglement but not in the least bound entanglement.

Looking again at table 6.2.3, one will notice that the outcomes of the SIC-witnesses concerning the first three five-parametric states are very similar, often even identical. This has occurred many times when employing the same witnesses on different states, regardless of the number of parameters or the precise composition of the states. As an example, consider the minimized expectation values of the SIC-witnesses for Kilian's state ρ_K and compare them to the results of $\rho_{1,5q}$, $\rho_{2,5q}$ or $\rho_{3,5q}$, see overall table 7.0.1.

Only the last of the four states characterized in this subsection presents different but unfortunately even worse values, probably again due to the very special structure of $\rho_{4,5q}$. But such strong deviations from the output data of the other states are very rare that is why listing them one time by $\rho_{4,5q}$ is enough to represent all of those exceptional cases which have been discovered so far.

Another riddle is the fact that all of the five-parametric states supply worse results for all SIC-witnesses than e.g. $\rho_{2,4q}$ from subsection 6.2.2. This does not depend on the number of parameters as we will see in the next chapter. So, is this behavior just a coincidence, meaning that not sufficient classes of states described by five parameters have been investigated to discover one with a similar output as $\rho_{2,4q}$ has provided? Naturally, this is easily possible, however, it is very remarkable that certain outcomes for the optimized expectation value such

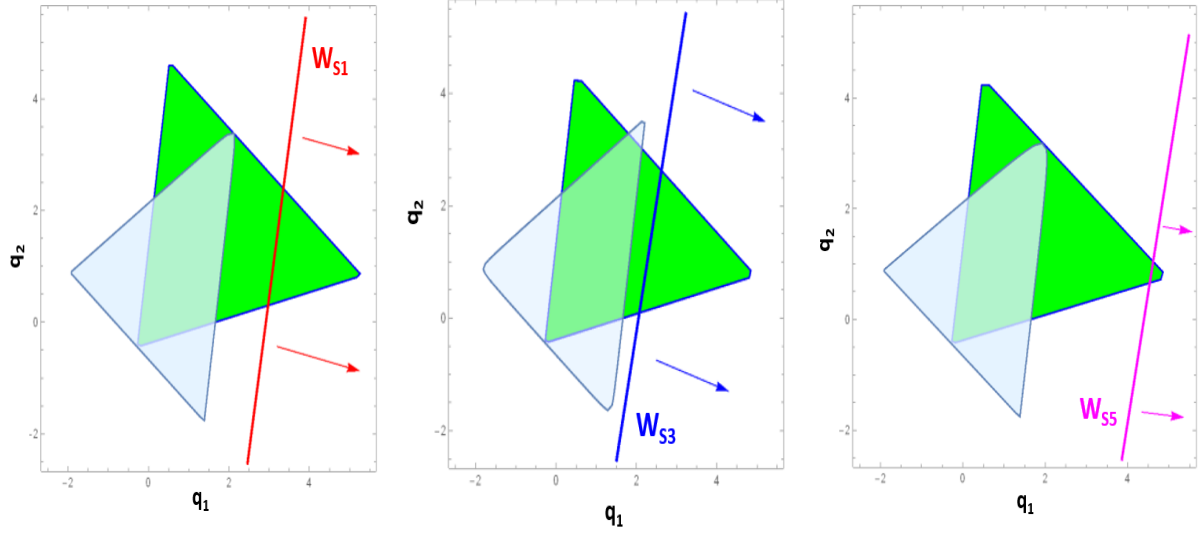


Figure 6.2.12: SIC-witnesses $\mathcal{W}_{S1} = W_{01}$ on $|s_1\rangle$ (left), $\mathcal{W}_{S3} = W_{02}$ on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ (central) and $\mathcal{W}_{S5} = W_{11}$ on $|s_1\rangle + W_{01}$ on $|s_2\rangle$ (right) applied to $\rho_{2,5q}$ plotted for q_1 and q_2 while the remaining parameters q_3 , q_4 and q_5 are fixed. The green triangle shows the field of positivity and the partly transparent blue one marks the range of PPT exposing the overlapping areas of positivity and PPT.

as 0.42967 for W_{01}/W_{02} on $|s_1\rangle$ show up for many different families of states exploiting different numbers of parameters such as $\rho_{1,5q}$ and ρ_K . Thus, a simple coincidence is unlikely; one can conclude that, compared to MUB-witnesses, the efficacy of SIC-witnesses is more heavily dependent on the given state.

6.2.4 Six and more Parameters

We now increase the number of parameters labeling the families of states structured within the magic simplex even further. Starting with six parameters, we finally go up to nine so that every Bell projector in the simplex is weighted by its own coefficient q_j . Enumerating the states is not necessary here since only one class of states is analyzed for each number of parameters, beginning with ρ_{6q} . Hence, in this chapter four families of states will be discussed and then the same MUB- and SIC- witnesses as given in table 6.2.1 are applied to them as we have already done in the last section. As a matter of fact, those witnesses have generally rendered the best outcomes, i.e. they have detected the most entanglement and bound entanglement, but they also represent very well many other witnesses tested throughout this thesis with similar findings. After optimizing the output data, all the results concerning witnesses and states are summarized in one table in order to provide a good overview.

Among the six-parametric states which have been investigated, the following one is outstanding due to its notable outcomes for both MUB- and SIC-witnesses:

$$\begin{aligned} \rho_{6q} = & \left(1 - \sum_{j=1}^6 q_j\right) \frac{1}{d^2} \mathbb{1}_{d^2} + q_1 P_{00} + \frac{q_2}{d-1} \sum_{i=1}^{d-1} P_{i0} + q_3 P_{01} + \frac{q_4}{d-1} \sum_{i=1}^{d-1} P_{i1} + \\ & + q_5 P_{02} + \frac{q_6}{d-1} \sum_{i=1}^{d-1} P_{i2}. \end{aligned} \quad (6.30)$$

The first horizontal phase space line is divided into three parameters, one for each Bell projector P_{kl} , while the remaining q_j 's deal with the vertical lines above them, thus each of those covers two maximally entangled states.

Now we introduce a seventh parameter. Using six q_j 's to cover every projector in the first two vertical phase space lines, we use the last coefficient q_7 solely for the entire third one:

$$\rho_{7q} = \left(1 - \sum_{j=1}^7 q_j\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \sum_{i=0}^{d-1} q_{i+1} P_{i0} + \sum_{i=0}^{d-1} q_{i+4} P_{i1} + \frac{q_7}{d} \sum_{i=0}^{d-1} P_{i2}. \quad (6.31)$$

Graphic representations of the structures of state ρ_{6q} and ρ_{7q} in the magic simplex are given in figure 6.2.13. Since each Bell projector in the first two phase space lines is assigned its own parameter in state ρ_{7q} , their explicit marking is not required, therefore only the simple colour distinction is shown.

The next families of states ρ_{8q} and ρ_{9q} with eight and nine parameters are not illustrated because they constitute just an extension of ρ_{7q} . In ρ_{8q} the last vertical line is set up by an unequal combination of the P_{kl} using q_7 and another parameter q_8 :

$$\rho_{8q} = \left(1 - \sum_{j=1}^8 q_j\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \sum_{i=0}^{d-1} q_{i+1} P_{i0} + \sum_{i=0}^{d-1} q_{i+4} P_{i1} + \frac{q_7}{d-1} \sum_{i=0}^{d-2} P_{i2} + q_8 P_{22}. \quad (6.32)$$



Figure 6.2.13: Graphical representation of the $\{P_{kl}\}_{k,l=0}^{d-1}$ distributed among parameters $\{q_j\}_{j=1}^6$ and $\{q_j\}_{j=1}^7$ forming the states ρ_{6q} (left) and ρ_{7q} (right) in the magic simplex.

And finally, we look at the case when there are nine parameters for nine Bell states. This class of states enables ultimate mixing of the maximally entangled states, so will it supply the best results for bound entanglement detection? For both MUB- and SIC-witnesses?

$$\rho_{9q} = \left(1 - \sum_{j=1}^9 q_j\right) \frac{1}{d^2} \mathbb{1}_{d^2} + \sum_{i=0}^{d-1} q_{i+1} P_{i0} + \sum_{i=0}^{d-1} q_{i+4} P_{i1} + \sum_{i=0}^{d-1} q_{i+7} P_{i2}. \quad (6.33)$$

We proceed with table 6.2.4 containing the output data of the most relevant witnesses for the states described above. The table is again structured the same way as table 6.2.1 with the same conventions for "+" and "/" and the optimized expectation values such as $\langle \mathcal{W}_{opt} \rangle_{\rho_{6q}}$ are again just noted ρ_{6q} .

Naturally, much more than just this couple of witnesses and far more than just one state per number of parameters have been checked, but for comparison purposes only those with the best or at least very surprising results are analyzed here.

Starting our analysis with MUBs, we can see that the as yet best witnesses, $\mathcal{W}_{M1}/\mathcal{W}_{M2} = W_{01}/W_{02}$ on B_1 , work perfectly again, but the other witnesses have improved as well compared to the classes of states we have discussed so far. Apart from the last MUB-witness listed in table 6.2.4, each of them is able to detect at least somewhat bound entanglement. Interestingly, the minimized expectation value decreases if the same witnesses are applied to states defined via more parameters. Take for an example W_{01} on B_4 used on ρ_{6q} , ρ_{7q} and ρ_{8q} and compare its output: The value becomes smaller and thereby increasing the detection efficiency although it is still quite weak compared to the performance of the same witness on the last state ρ_{9q} equipped with the maximum number of parameters.

Apparently, the number of parameters is crucial for finding bound entanglement employing MUB-witnesses. State ρ_{8q} already gives great results for witnesses like W_{01}/W_{02} on B_3/B_4 that have not been very successful up to now. But even this progress seems little if one looks at the outcomes of ρ_{9q} where every MUB-witness except for the last one is capable of detecting the same amount of bound entanglement as $\mathcal{W}_{M1}/\mathcal{W}_{M2}$ does. Can this success be simply explained by the nine parameters, i.e. one parameter for each Bell projector, which provide mximal mixing and weighting those? For witnesses like W_{01}/W_{02} on B_3 this assumption appears logical since we have a steady reduction of the optimized expectation value if we go from ρ_{6q} to ρ_{9q} . But for other witnesses like W_{01} on B_4 , we have a jump in detection efficiency that seems to appear from nowhere. Other witnesses such as

Optimized witnesses $\mathcal{W}_{opt}$	ρ_{6q}	ρ_{7q}	ρ_{8q}	ρ_{9q}
W_{01} / W_{02} on B_1	-0.1547	-0.1547	-0.1547	-0.1547
W_{01} / W_{02} on B_3	-0.02073	-0.02252	-0.13909	-0.1547
W_{01} on B_4	-0.02073	-0.02252	-0.03688	-0.1547
W_{02} on B_4	-0.02073	-0.02252	-0.1547	-0.1547
W_{01} on $(B_2 + B_3) +$ $+ W_{02}$ on $(B_1 + B_4)$	-0.02073	-0.02252	-0.03688	-0.1547
W_{12} on $B_1 + W_{21}$ on $B_2 +$ $+ W_{11}$ on $B_3 + W_{22}$ on B_4	0	0	0	0
W_{01} on $ s_1\rangle$	0.375	0.42967	0.41616	0.375
W_{02} on $ s_1\rangle$	0.375	0.42636	0.41421	0.375
W_{01} on $(s_1\rangle + s_2\rangle)$	0.41073	0.51768	0.49168	0.41073
W_{02} on $(s_1\rangle + s_2\rangle)$	0.41073	0.50369	0.48284	0.41073
W_{01} on $ s_1\rangle + W_{02}$ on $ s_2\rangle$	0.44075	0.54772	0.5217	0.44074
W_{02} on $ s_1\rangle + W_{11}$ on $ s_2\rangle$	0.50159	0.52524	0.50138	0.49922
W_{11} on $ s_1\rangle + W_{01}$ on $ s_2\rangle$	0.79523	0.81886	0.79523	0.79286
W_{01} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	0.375	0.48195	0.45595	0.375
W_{02} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	0.375	0.46796	0.44711	0.375
W_{02} on $ s_1\rangle + W_{01}$ on $ s_4\rangle /$ W_{01} on $ s_1\rangle + W_{02}$ on $ s_7\rangle /$				
W_{02} on $ s_4\rangle + W_{01}$ on $ s_7\rangle$	0	0.10698	0.08095	0
W_{01} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	0	0.15537	0.11847	0
W_{02} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	0	0.12291	0.09626	0

Table 6.2.4: Optimized expectation values calculated for a selection of MUB- and SIC-witnesses applied to states ρ_{6q} , ρ_{7q} , ρ_{8q} and ρ_{9q} . All results $\leq |\pm 10^{-7}|$ are rounded to zero.

W_{12} on $B_1 + W_{21}$ on $B_2 + W_{11}$ on $B_3 + W_{22}$ on B_4 obviously never work, not even for the best state available, maybe because they are too complicated - too many Weyl operators and MUBs involved.

In figure 6.2.14 two graphical plots are given to show the distinction in capability to detect bound entanglement for one and the same witness, W_{01} on $B_4 = \mathcal{W}_{M4}$, applied to two states with a different number of parameters: ρ_{8q} and ρ_{9q} . While the cut through the magic simplex for ρ_{8q} in the left image only shows quite a small detection power, the situation looks completely different in the right plot: For ρ_{9q} , the region of bound entanglement is huge compared to the output of the same witness employed on the state with just one parameter less.

According to all of the findings of MUB-witnesses treated so far, one can conclude that, in general, more of them are able to reveal bound entanglement and their detection performance is raised if the number of parameters characterizing the states is increased. This aspect can be seen in table 6.2.4, but also when comparing its numeric data to those shown in the previous tables listing the four- and five-parametric families of states (see overall table 7.0.1).

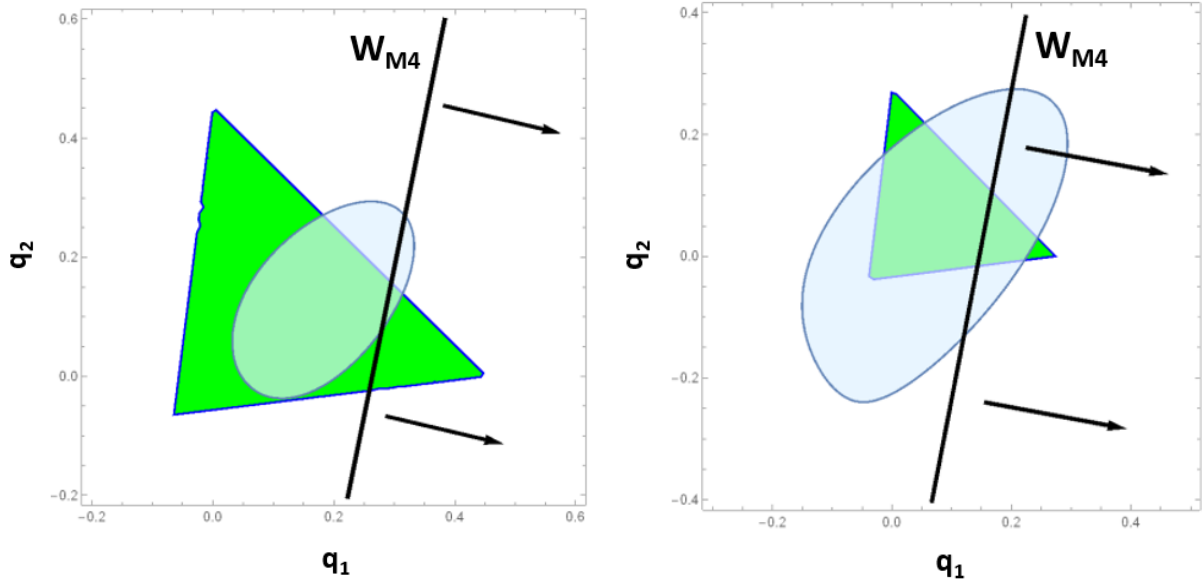


Figure 6.2.14: MUB-witness $\mathcal{W}_{M4} = W_{01}$ on B_4 applied to both ρ_{8q} (left) and ρ_{9q} (right) plotted for parameters q_1 and q_2 while the remaining parameters are fixed. The green triangle represents the region of positivity and the light blue, partially transparent oval marks the field of PPT. The small area where positivity and PPT overlap and which is exposed by the witness, constitutes the zone of bound entanglement.

At first view, the dependence of good or better results on the number of parameters does not seem to hold for SIC-witnesses. While ρ_{6q} and ρ_{9q} give the best expectation values since $\rho_{2,4q}$, the states with seven or eight parameters yield worse outcomes, but they are remarkably similar to those of most five-parametric states, such as $\rho_{1,5q}$, $\rho_{2,5q}$ or $\rho_{3,5q}$ in table 6.2.3. However, if one takes a more detailed look at these findings, one can notice that the output data of the optimized SIC-witnesses used on ρ_{7q} is in general slightly improved compared to states like e.g. $\rho_{2,5q}$. And the values of ρ_{8q} are again distinctly smaller than those of ρ_{7q} - take again a look at the large table 7.0.1 at the end of the thesis for comparisons. Hence, for both MUB- and SIC-witnesses, their detection efficiency of bound entanglement is at least partially dependent on the number of parameters used in the states the witnesses are applied to.

Nonetheless, choosing an appropriate class of states with a certain mixing of the maximally entangled states is obviously more important if one wants to attain the best results for SIC-witnesses that could have been found within the scope of this thesis. States such as $\rho_{2,4q}$ or ρ_{6q} apparently demonstrate a non-dependence on the number of parameters. However, for ρ_{9q} which also provides the same outcomes, the crucial point seems here the maximal number of parameters possible (as it is for the output of the MUB-witnesses) since this state obviously does not have any special composition. Examining the expectation values of the SIC-witnesses W_{01} on $|s_1\rangle + W_{02}$ on $|s_2\rangle$, W_{02} on $|s_1\rangle + W_{11}$ on $|s_2\rangle$ and W_{11} on $|s_1\rangle + W_{01}$ on $|s_2\rangle$ used on ρ_{9q} very carefully and comparing those to the values of ρ_{6q} or $\rho_{2,4q}$, one finds a very small improvement, within just a few thousandths (see table 7.0.1). Still, this can be considered as

another hint that the more parameters the states perform the more powerful the witnesses are.

In general, summing up the findings of all MUB- and SIC-witnesses applied to the individual families of states we have considered in this work, one finds that shifting the MUB- and SIC-vectors only (by utilizing W_{01} or W_{02}) without any phase shift frequently renders a better output than including one (by deploying roots of unity, ω). However, as we have already observed in the last section at state $\rho_{4,5q}$, this behavior of entanglement witnesses can vary significantly with the given state. Generally, if phases are included in the generated state, Weyl operators containing phases such as W_{11} , are important for the construction of entanglement witnesses since it is the product of witness and state (resulting in the expectation value) which determines the efficacy of the witness.

Again, the last five witnesses listed in table 6.2.4 provide the best results obtainable for the SIC-method. This time, the improvement effect of W_{02} compared to W_{01} is more significant and clearly recognizable when considering the outcomes of any SIC-witness on the states ρ_{7q} or ρ_{8q} , in particular the very last witness, W_{01}/W_{02} on $(|s_1\rangle + |s_4\rangle + |s_7\rangle)$.

In figure 6.2.15 two graphical plots displaying the witness $\mathcal{W}_{S3} = W_{02}$ on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ applied to two states with a different number of parameters are given: For ρ_{7q} and ρ_{8q} , this SIC-witness has turned out to be the most efficient one. Contrary to MUBs above in figure 6.2.14, having one parameter more does not necessarily mean much better results: $\mathcal{W}_{S3}$ on ρ_{8q} is hardly better than on ρ_{7q} , yet both of them miss the region of bound entanglement.

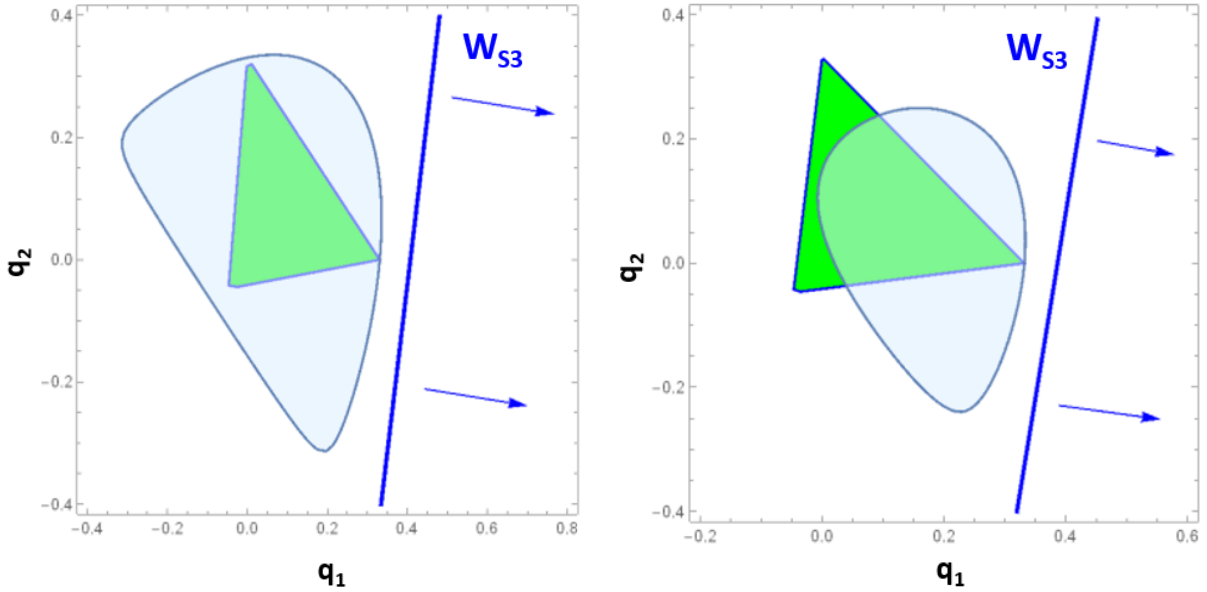


Figure 6.2.15: SIC-witness $\mathcal{W}_{S3} = W_{02}$ on $|s_1\rangle + W_{01}$ on $|s_4\rangle$ applied to both ρ_{7q} (left) and ρ_{8q} (right) plotted for q_1 and q_2 while the remaining parameters are fixed. While the green triangle shows the area of positivity, the light blue region marks the field of PPT.

Unfortunately, it has not been possible to create an appropriate plot for the states ρ_{6q} or ρ_{9q} , where a graphic visualization of a witness like $\mathcal{W}_{S3}$ would have been even more expressive.

In the end, we have not managed to detect any bound entanglement via SIC-witnesses. Even the most complex state with nine parameters providing excellent results employing MUB-witnesses does not show the slightest chance to find any PPT-entanglement using SICs. In the overall table 7.0.1, all findings of the most relevant SIC-witnesses (and also MUB-witnesses) employed on the main classes of states are presented.

What is the problem with SIC-witnesses? Optimized MUB-witnesses are successful in at least some cases and if they fail to detect any bound entanglement, they are still mostly close to it, resulting in an expectation value of zero. But only five SIC-witnesses have been found that managed to reach the boundary of the wanted bound entanglement detection, i.e. $\langle \mathcal{W} \rangle_\rho = 0$, and even that has only occurred if those witnesses are applied to three special families of states ($\rho_{2,4q}$, ρ_{6q} , ρ_{9q}). Why are the outcomes of SIC-witnesses in general much worse than of MUB-witnesses?

One explanation might be the fact that SIC-witnesses do not have a fixed upper bound on the set of separable states when local shifts (implemented by Weyl operators) are used for their construction. Unlike MUB-witnesses, this bound has to be computed for each SIC-witness individually and thus often varies significantly (see table 6.2.2). As already analyzed in subsection 6.2.2 there seems to be a correlation between the upper bound and the quality, i.e. the efficiency in entanglement detection, of the witness.

Maybe the problem (or one of the problems) is the different structure of SIC-POVM elements, given by nine SIC-vectors (for $d = 3$), and MUBs, represented by four bases each consisting of three vectors. This may cause a more sophisticated context if they are exploited in witness construction applied to a heavily mixed state used on a phase space setup. That is, there may exist some further, more subtle, deeper-lying relationships between MUBs and SICs we do not understand yet.

7 Conclusion

This thesis gives a comparison between two different types of entanglement witnesses concerning their ability of detecting bound entanglement in bipartite qutrit systems: First, employing a complete set of Mutually Unbiased Bases (MUBs) and, second, using Symmetric Informationally Complete Positive Operator-Valued Measures (SIC-POVMs) to constitute the witnesses which are then applied to various classes of states. Out of all the witnesses and states tested for this study, the most promising and most representative ones have been chosen to be discussed in order to provide a concise overview and to make a comparison of them as expressive as possible. A summary of all these outcomes is given in the overall table 7.0.1 on page 63. The families of states are embedded within a discrete classical phase space showing high symmetries, the so-called magic simplex, thus they are characterized by d^2 Bell projectors and a certain number of parameters which has been varied several times.

The entanglement witnesses have been constructed by using correlations functions where Weyl operators are employed on different MUBs or SIC-vectors in the second subsystem (Bob's subsystem). It has turned out that witnesses created by Weyl shifts W_{01} and W_{02} rearranging the vectors in the first MUB B_1 in the correlation function usually yield by far the best results when applied to any family of states. The maximum amount of bound entanglement which can be found by MUB-witnesses in bipartite qutrit systems seems to be restricted to $1 - \frac{2}{\sqrt{3}} \approx -0.1547$ since not a single witness employed on any state has ever yielded better expectation values. States using more parameters can enhance the chance to reveal bound entanglement, in particular for other MUB-witnesses than those formed by W_{01} or W_{02} on B_1 , thus showing that bound entangled states are indeed highly mixed states.

The application of witnesses generated by a full set of MUBs has been in general successful, however, all witnesses established via the SIC-POVM have turned out to be much less effective in finding regions of bound entanglement. Apparently, this remarkable behavior of SIC-witnesses does not depend on the states they are applied to. From that we conclude that the reasons for this have to lie in the structure of these witnesses. On the other hand, looking at the output of all the optimized SIC-witnesses in table 7.0.1 one can recognize a clear dependence on the considered state and thereby on the magic simplex and its symmetries, which is even more distinctive than using MUB-witnesses. One explanation for this observation might be the fact that the upper bound on the set of separable states is not independent of the particular SIC-witness if Weyl operators are employed on single SIC-vectors. So this bound is very variable even for a complete set of SICs while it is fixed for MUBs, that is, for a total set of MUBs, the MUB-criterion does not depend on any local shift on MUBs. This is an important difference between the MUB- and SIC-criterions.

Furthermore, it has been shown that for MUB- and SIC-witnesses, respectively, only shifting MUB- and SIC-vectors, i.e. applying W_{01} or W_{02} , without any phase shift does render better results. Deploying any root of unity in the witness construction apparently decreases the efficiency of it significantly, e.g. using W_{kl} with $k \neq 0$ or MUBs other than B_1 or SIC-vectors other than $|s_1\rangle$, $|s_4\rangle$ or $|s_7\rangle$. However, this effect could be explained by the chosen families of states, since for all of them different Bell projectors P_{kl} , defined via W_{kl} , have been exploited.

And there are exceptions like $\rho_{4,5q}$, the outcomes of which obviously show that this property can indeed depend on the given state - the MUB-witnesses indicate here the opposite behavior.

Moreover, changing the parameterization of a state just slightly, meaning that choosing a somewhat different distribution of the parameters among the Bell projectors and/or adding another parameter to the state often provides quite contrasting results for many MUB- and SIC-witnesses, e.g. comparing ρ_{8q} and ρ_{9q} in table 7.0.1.

Summing up the findings of all MUB- and SIC-witnesses applied to the classes of states which this thesis has covered, one can conclude that local shifts on the vectors within MUBs enable detection of bound entanglement, while this does not hold for any local shift on SIC-vectors. A full set of MUBs and SICs are different but equivalent concepts in the sense that they are both quantum 2-designs. And both of them serve as useful tools in quantum information science and can be easily implemented in the laboratory. Still, an experimenter cannot choose one of the two methods arbitrarily for a quantum detection test - if they want to detect bound entanglement, SICs are obviously not as suitable as MUBs. It is important for the researcher to take this fact into account when planning an experiment dealing with MUBs or SICs.

However, SIC-witnesses generally vary stronger in the minimized expectation value and show state-dependence when local shifts are used for witness construction. The same witnesses operating on certain families of states can provide far better outcomes than on other ones despite of their similar structures in the magic simplex. That behavior of SIC-witnesses indicates a higher dependency on the symmetry of the magic simplex than MUB-witnesses. For future purposes and applications, e.g., in specialized quantum protocols, this observation might turn out to be handy and auspicious.

The apparent inability of witnesses formed by the Hesse-SICs to detect any bound entanglement is definitely an issue which requires further research. A further research line could be the comparison between MUB- and SIC-witnesses on detection of bound entanglement towards higher dimensions in bipartite or even multipartite quantum systems. This might also shed some light on possibly yet unknown structures of MUBs and SIC-POVMs and especially on the relationships between them. Trying to confirm the results of SIC-witnesses in this thesis by utilizing a different construction method of SIC-POVMs could also be of interest - maybe other than the Hesse-SIC construction can achieve better outcomes. In addition, this thesis treated linear entanglement witnesses working with the upper bound on the set of separable states, thus a careful study of the lower bound and of non-linear MUB- and SIC-witnesses (or even a combination of both) would be a very intriguing research task.

Optimized witnesses $\mathcal{W}_{opt}$	ρ_K	$\rho_{2,4q}$	$\rho_{1,5q}$	$\rho_{2,5q}$	$\rho_{3,5q}$	$\rho_{4,5q}$	ρ_{6q}	ρ_{7q}	ρ_{8q}	ρ_{9q}
W_{01} / W_{02} on B_1	-0.1547	0	-0.1547	-0.1547	-0.1547	0.40457	-0.1547	-0.1547	-0.1547	-0.1547
W_{01} on B_3	0	0	0	-0.01342	0	0.19098	-0.02073	-0.02252	-0.13909	-0.1547
W_{02} on B_3	0	0	0	0	0	0.2	-0.02073	-0.02252	-0.13909	-0.1547
W_{01} on B_4	0	0	0	0	-0.01342	0	-0.02073	-0.02252	-0.03688	-0.1547
W_{02} on B_4	0	0	0	0	0	0.0623	-0.02073	-0.02252	-0.1547	-0.1547
W_{01} on $(B_2 + B_3) +$ $+ W_{02}$ on $(B_1 + B_4)$	0	0	0	0	0	0.10539	-0.02073	-0.02252	-0.03688	-0.1547
W_{12} on $B_1 + W_{21}$ on $B_2 +$ $+ W_{11}$ on $B_3 + W_{22}$ on B_4	0	0	0	0	0	0	0	0	0	0
W_{01} on $ s_1\rangle$	0.42967	0.375	0.42967	0.42967	0.42967	0.56067	0.375	0.42967	0.41616	0.375
W_{02} on $ s_1\rangle$	0.42967	0.375	0.42967	0.42884	0.42884	0.5652	0.375	0.42636	0.41421	0.375
W_{01} on $(s_1\rangle + s_2\rangle)$	0.51768	0.41073	0.51768	0.51768	0.51768	0.63328	0.41073	0.51768	0.49168	0.41073
W_{02} on $(s_1\rangle + s_2\rangle)$	0.51768	0.41073	0.51768	0.51413	0.51413	0.62914	0.41073	0.50369	0.48284	0.41073
W_{01} on $ s_1\rangle + W_{02}$ on $ s_2\rangle$	0.55186	0.44075	0.55186	0.55082	0.55082	0.67495	0.44075	0.54772	0.5217	0.44074
W_{02} on $ s_1\rangle + W_{11}$ on $ s_2\rangle$	0.52938	0.5016	0.52938	0.52834	0.52834	0.66006	0.50159	0.52524	0.50138	0.49922
W_{11} on $ s_1\rangle + W_{01}$ on $ s_2\rangle$	0.81886	0.79524	0.81886	0.81886	0.81886	0.95311	0.79523	0.81886	0.79523	0.79286
W_{01} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	0.48195	0.375	0.48195	0.48195	0.48195	0.59755	0.375	0.48195	0.45595	0.375
W_{02} on $(s_1\rangle + s_4\rangle / s_7\rangle)$	0.48195	0.375	0.48195	0.4784	0.4784	0.5934	0.375	0.46796	0.44711	0.375
W_{02} on $ s_1\rangle + W_{01}$ on $ s_4\rangle /$ W_{01} on $ s_1\rangle + W_{02}$ on $ s_7\rangle /$	0.11111	0	0.11111	0.11007	0.11007	0.2342	0	0.10698	0.08095	0
W_{02} on $ s_4\rangle + W_{01}$ on $ s_7\rangle$	0.15537	0	0.15537	0.15537	0.15537	0.25	0	0.15537	0.11847	0
W_{01} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	0.15537	0	0.15537	0.14694	0.14694	0.22805	0	0.12291	0.09626	0
W_{02} on $(s_1\rangle + s_4\rangle + s_7\rangle)$	0.15537	0	0.15537	0.14694	0.14694	0.22805	0	0.12291	0.09626	0

Table 7.0.1: Expectation values of some MUB-witnesses (upper part) and SIC-witnesses (lower part), minimized over all parameters, listed for all relevant families of states presented in this thesis: ρ_K , $\rho_{2,4q}$, $\rho_{1,5q}$, $\rho_{2,5q}$, $\rho_{3,5q}$, $\rho_{4,5q}$, ρ_{6q} , ρ_{7q} , ρ_{8q} and ρ_{9q} . If a

Weyl operator is applied to more than one MUB or SIC-vector, we mark such a combination by "+" while "/" indicates that either this operator (or combination of operators) or the other one can be used generating identical results. MUB- and SIC-witnesses are separated by the horizontal double line at the center of the table. All results $\leq |\pm 10^{-7}|$ are rounded to zero.

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