Abstract

We present a study of extremal entanglement witnesses on a bipartite composite quantum system. We define the cone of entanglement witnesses as the dual of the cone of unnormalized separable density matrices, this means that $\text{Tr} \Omega \rho \geq 0$ whenever $\Omega$ is a witness and $\rho$ is a pure product state, $\rho = \psi \psi^\dagger$ with $\psi = \phi \otimes \chi$. The set of witnesses normalized to unit trace is a compact convex set, uniquely defined by its extremal points. Therefore we want to study these extremal witnesses. We use numerical methods because this enables us to handle all witnesses. The expectation value $\text{Tr} \Omega \rho$ as a function of vectors $\phi$ and $\chi$ is a positive semidefinite biquadratic form. Every zero of a positive biquadratic form imposes strong real-linear constraints on the form. In every direction at the zero the first derivative must vanish and the second derivative must be nonnegative. If the second derivative vanishes, the third derivative must vanish and the fourth derivative must be nonnegative. The Hessian matrix at the zero, which is real and symmetric, must be positive semidefinite. The eigenvectors of the Hessian with zero eigenvalue, if such exist, we call Hessian zeros. A zero of the biquadratic form is called quadratic if it has no Hessian zeros, otherwise it is called quartic. We call a witness quadratic if it has only quadratic zeros, and quartic if it has at least one quartic zero. A main result we prove is that a witness is extremal if and only if no other witness has the same set, or a larger set, of zeros and Hessian zeros.

We use the complete set of constraints defined by the zeros and Hessian zeros of a witness in order to test for extremality. If the witness is not extremal, the test gives all the directions in the space of Hermitian matrices in which we may search for witnesses that have more zeros or Hessian zeros and hence are more nearly extremal. A finite number of iterated searches in random directions lead to an extremal witness which is nearly always quadratic, with a fixed minimum number of isolated zeros depending on the Hilbert space dimensions. In spite of the fact that extremal witnesses of this type are by far the most common, it seems that they have never been described in the literature. Previously known extremal witnesses all have continuous sets of quartic zeros.

We discuss briefly some topics related to extremal witnesses, in particular the relation between the facial structures of the dual sets of witnesses and separable states. We discuss the relation between extremality and optimality of witnesses, and a special conjecture of separability of the so called structural physical approximation (SPA) of an optimal witness. Finally, we point out the possibility of treating the entanglement witnesses on a complex Hilbert space as a subset of the witnesses on a real Hilbert space.
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1 Introduction

Entanglement is the quintessence of nonclassicality in composite quantum systems. As a physical resource it finds many applications especially in quantum information theory, see [1,2] and references therein. Entangled states are exactly those states that can not be modelled within the classical paradigm of locality and realism [3–6]. Contrary to states of classical composite systems, they allow better knowledge of the system as a whole than of each component of the system [7,8]. The notion of entanglement is therefore of interest within areas of both application and interpretation of quantum mechanics.

The problem of distinguishing entangled states from nonentangled (separable) states is a fundamental issue. Pure separable states of a bipartite system are exactly the pure product states, they are easily recognized by singular value decomposition, also known as Schmidt decomposition [2]. The situation is much more complicated for mixed states. A separable mixed state is a state mixed from pure product states [5].

The separability problem of distinguishing mixed separable states from mixed entangled states has received attention along two lines. On the one hand, operational or computational tests for separability are constructed [9]. On the other hand, the geometry of the problem is studied, with the aim of clarifying the structures defining separability [10–18]. Two results, one from each approach, deserve special attention. An operationally simple necessary condition for separability was given by Peres [9]. He pointed out that the partial transpose of a separable state is again a separable state, therefore we know that a state is entangled if its partial transpose is not positive semidefinite. States with positive partial transpose, so called PPT states, are interesting in their own right [19]. A significant geometrical result is that of Życzkowski et al. that the volume of separable states is nonzero [12]. They prove the existence of a ball of separable states surrounding the maximally mixed state. The maximal radius of this ball was provided by Gurvits and Barnum [13].

The well known necessary and sufficient separability condition in terms of positive linear maps or entanglement witnesses connects these two lines of thought [11,20]. There exists a set of linear maps on states, or equivalently a set of observables called entanglement witnesses, that may detect, or witness, entanglement of a state. This result is the point of departure for almost all research into the problem, be it computational, operational or geometrical. The
major obstacle in the application of positive linear maps and entanglement witnesses is that they are difficult to identify, in principle as difficult as are the entangled states themselves.

Our contribution falls in the line of geometrical studies of entanglement. The ultimate goal is to classify the extremal points of the convex set of entanglement witnesses, the building blocks of the set, in a manner useful for purposes in quantum mechanics. Positive linear maps, and the extremal positive maps, were studied already in 1963 by Størmer in the context of partially ordered vector spaces and \( C^* \) algebras [14,15]. Since then the extremal positive maps and extremal witnesses have only received scattered attention [21–28].

Here we combine and apply basic notions from convex geometry and optimization theory in order to study the extremal entanglement witnesses. We obtain computationally useful necessary and sufficient conditions for extremality. We use these ideas to analyse previously known examples and construct new numerical examples of extremal witnesses. The extremal witnesses found in random searches are generic, by definition. It turns out that the previously known examples of extremal witnesses are very far from being generic, and the generic extremal witness is of a type not yet published in the literature.

We discuss what we learn about the geometry of the set of witnesses, and also the set of separable states, by studying extremal witnesses. Other topics we comment on are the relation between extremal and optimal witnesses [26,29], and the so called structural physical approximation (SPA) of witnesses relating them to physical maps of states [30–32].

Numerical methods play a central role in our work. An important reason is that the entanglement witnesses we want to study are so complicated that there is little hope of treating them analytically. Numerical work is useful for illustrating the theory, examining questions of interest and guiding our thoughts in questions we cannot answer rigorously.

The methods we use for studying extremal witnesses are essentially the same as we have used previously for studying extremal states with positive partial transpose (PPT states) [18, 33–36]. The work presented here is also based in part on the master’s thesis of one of us [37].

Outline of the article

This article consists of three main parts. Section 2 is the first part, where we review material necessary for the appreciation of later sections. The basic concepts of convex geometry are indispensable. We review the geometry of entanglement witnesses, and formulate the study of extremal witnesses as an optimization problem where we represent the witness as a positive semidefinite biquadratic form and study its zeros.

The second part consists of Section 3 and Section 4, where we develop a necessary and sufficient condition for the extremality of a witness. The basic idea is that every zero of a positive biquadratic form representing a witness imposes strong linear constraints on the form. The extremality condition in terms of the zeros of a witness and the associated constraints is our most important result, not only because it gives theoretical insight, but because it is directly useful for numerical computations.

In the third, last, and most voluminous part, the Sections 5 to 11, we apply the extremality condition from Section 4. As a first application we study decomposable witnesses in Section 5. These are well understood and not very useful as witnesses, since they can only detect the entanglement of a state in the trivial case when its partial transpose is not positive. But they serve to illustrate the concepts, and we find them useful as stepping stones towards nondecomposable witnesses.

In Section 6 we study examples of extremal nondecomposable witnesses. First we study
two examples known from the literature, and confirm their extremality by our numerical method. Then we construct numerically random examples of extremal witnesses in order to learn about their properties. We find that the generic extremal witnesses constructed numerically belong almost without exception to a completely new class, not previously noticed in the literature. They have a fixed number of isolated quadratic zeros, whereas the previously published extremal witnesses have continuous sets of zeros. The number of zeros depends on the dimensions of the Hilbert spaces of the two subsystems.

In Section 7 we show examples of a special D-shaped type of faces of the set of witnesses in the lowest nontrivial dimensions, $2 \times 4$ and $3 \times 3$. These faces are “next to extremal”, bordered by extremal witnesses plus a straight section of decomposable witnesses.

In Section 8 we study faces of the set of separable states, using the duality between separable states and witnesses. We classify two different families of faces, generalizing results of Alfsen and Shultz [16], and present some statistics on randomly generated maximal simplex faces. We point out that the facial structure is relevant for the question of how many pure product states are needed in the convex decomposition of an arbitrary separable state, and suggest that it may be possible to improve substantially the trivial bound given by the dimension of the set [38, 39].

In Section 9 we compare the notions of optimal and extremal witnesses [26, 29]. In low dimensions we find that almost every nondecomposable optimal witness is extremal, whereas an abundance of nondecomposable and nonextremal optimal witnesses exist in higher dimensions.

In Section 10 we comment on a separability conjecture regarding structural physical approximations (SPAs) of optimal witnesses [30, 31]. This conjecture has since been refuted [32, 40]. We have tried to test numerically a modified separability conjecture. It holds within the numerical precision of our separability test, but this test with the available precision is clearly not a definitive proof.

In Section 11 we point out that it is possible, and maybe even natural from a certain point of view, to treat the entanglement witnesses on a complex tensor product space as a subset of the witnesses on a real tensor product space.

In Section 12 we summarize our work and suggest some possible directions for future efforts. Some details regarding numerical methods are found in the Appendix.

2 Background material

In this section we review material necessary as background for the following sections. Convex geometry is the mathematical basis of the theory of mixed quantum states, and is equally basic in the entanglement theory for mixed states. We introduce the concepts of dual convex cones, entanglement witnesses, positive maps, and biquadratic forms. See e.g. introductory sections of [10] or [41] for further details on convexity. Concepts from optimization theory are useful in the numerical treatment of a special minimization problem, see [41, 42].

2.1 Convexity

The basic concepts of convex geometry are useful or even essential for describing mixed quantum states as probabilistic mixtures of pure quantum states. A convex subset of a real affine space is defined by the property that any convex combination

$$x = (1 - p)x_1 + px_2 \quad \text{with} \quad 0 \leq p \leq 1$$

(1)
of members \(x_1, x_2\) is a member. If \(x_1 \neq x_2\) and \(0 < p < 1\) we say that \(x\) is a proper convex combination of \(x_1, x_2\), and \(x\) is an interior point of the line segment between \(x_1\) and \(x_2\).

The dimension of a convex set is the dimension of the smallest affine space containing it. We will be dealing here only with finite dimensional sets. Closed and bounded subsets of finite dimensional Euclidean spaces are compact, according to the Heine–Borel theorem. A compact convex set has extremal points that are not convex combinations of other points. It is completely described by its extremal points, since any point in the set can be decomposed as a convex combination involving no more than \(n + 1\) extremal points, where \(n\) is the dimension of the set [39]. It is called a polytope if it has a finite number of extremal points, and a simplex if the number of extremal points is one more than the dimension.

**Definition 2.1.** A bidirection at \(x\) in the convex set \(K\) is a direction vector \(v \neq 0\) such that \(x + tv \in K\) for \(t\) in some interval \([t_1, t_2]\) with \(t_1 < 0 < t_2\).

A face \(F\) of \(K\) is a convex subset of \(K\) with the property that if \(x \in F\) then every bidirection in \(K\) at \(x\) is a bidirection in \(F\) at \(x\).

An equivalent condition defining \(F\) as a face is that if \(x \in F\) is a proper convex combination of \(x_1, x_2 \in K\), then \(x_1, x_2 \in F\).

The empty set and \(K\) itself are faces of \(K\), by definition. All other faces are called proper faces. The extremal points of \(K\) are the zero dimensional faces of \(K\). A face of dimension \(n - 1\) where \(n\) is the dimension of \(K\) is called a facet.

A point \(x\) in a convex set \(K\) is an interior point of \(K\) if every direction at \(x\) (in the minimal affine space containing \(K\)) is a bidirection, otherwise \(x\) is a boundary point of \(K\). Every point \(x \in K\) is either an extremal point of \(K\) or an interior point of a unique face \(F_x\) of dimension one or higher. This face is the intersection of \(K\) with the affine space

\[
A_x = \{ x + tv \mid t \in \mathbb{R}, v \in B_x \}
\]

where \(B_x\) is the set of all bidirections in \(K\) at \(x\).

Thus, every face \(F\) of \(K\) is an intersection \(F = A \cap K\) of \(K\) with some affine space \(A\). We take \(A\) to be a subspace of the minimal affine space containing \(K\). The minimum dimension of \(A\) is the dimension of \(F\), but it may also be possible to choose \(A\) as an affine space of higher dimension than \(F\). A proper face \(F = A \cap K\) is said to be exposed if \(A\) has dimension \(n - 1\) where \(n\) is the dimension of \(K\). Note that an exposed face may have dimension less than \(n - 1\), thus it is not necessarily a facet, and it may be just a point. Every exposed point is extremal, since it is a zero dimensional face, but a convex set may have extremal points that are not exposed.

A proper face of \(K\) is part of the boundary of \(K\). The faces of a face \(F\) of \(K\) are the faces of \(K\) contained in \(F\). In particular, the following result is useful for understanding the face structure of a convex set when its extremal points are known.

**Theorem 2.1.** Let \(F\) be a face of the convex set \(K\). Then a point in \(F\) is an extremal point of \(F\) if and only if it is an extremal point of \(K\).

We state here another useful result which follows directly from the definitions.

**Theorem 2.2.** An intersection \(K = K_1 \cap K_2\) of two convex sets \(K_1\) and \(K_2\) is again a convex set, and every face \(F\) of \(K\) is an intersection \(F = F_1 \cap F_2\) of faces \(F_1\) of \(K_1\) and \(F_2\) of \(K_2\).
The facial structure of \( \mathcal{K} = \mathcal{K}_1 \cap \mathcal{K}_2 \) follows from Definition 2.1 because the bidirections at any point \( x \in \mathcal{K} \) are the common bidirections at \( x \) in \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \).

A cone \( \mathcal{C} \) in a real vector space is a set such that if \( x \in \mathcal{C}, \ x \neq 0 \), then \( tx \in \mathcal{C} \) but \( -tx \notin \mathcal{C} \) for every \( t > 0 \). The concept of dual convex cones, to be defined below, has found a central place in the theory of quantum entanglement.

### 2.2 Quantum states

We are concerned here with a bipartite quantum system with Hilbert space \( \mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b \) of finite dimension \( N = N_a N_b \). The real vector space \( \mathcal{H} \) of observables on \( \mathcal{H} \) has dimension \( N^2 \), a natural Euclidean inner product \( \langle A, B \rangle = \text{Tr} \ A B \) and the corresponding Hilbert–Schmidt norm \( \|A\| = \sqrt{\text{Tr} \ A^2} \). We take \( \mathcal{H}_a = \mathbb{C}^{N_a}, \mathcal{H}_b = \mathbb{C}^{N_b} \), so \( \mathcal{H} \) is the set of Hermitian matrices in the matrix algebra \( M_N(\mathbb{C}) \). We write the components of a vector \( \psi \in \mathbb{C}^N \) as \( \psi_I = \psi_{ij} \) with \( I = 1, 2, \ldots, N \) or \( ij = 11, 12, \ldots, N_a N_b \). For any \( A \in \mathcal{H} \) we define \( A^\dagger \) as the partial transpose of \( A \) with respect to the second subsystem, that is,

\[
(A^\dagger)_{ij;kl} = A_{il;kj}.
\]

The set of positive semidefinite matrices in \( \mathcal{H} \) is a closed convex cone which we denote by \( \mathcal{D} \). The state space of the quantum system is the intersection \( \mathcal{D}_1 \) between \( \mathcal{D} \) and the hyperplane defined by \( \text{Tr} \ A = 1 \). The matrices in \( \mathcal{D}_1 \) are called density matrices, or mixed quantum states. A vector \( \psi \in \mathcal{H} \) with \( \psi^\dagger \psi = 1 \) defines a pure state \( \psi \psi^\dagger \in \mathcal{D}_1 \). \( \mathcal{D}_1 \) is a compact convex set of dimension \( N^2 - 1 \). The pure states are the extremal points of \( \mathcal{D}_1 \), in fact this is an alternative definition of \( \mathcal{D}_1 \).

A pure state \( \psi \psi^\dagger \) is separable if \( \psi \) is a product vector, \( \psi = \phi \otimes \chi \), thus a separable pure state is a tensor product of pure states,

\[
\psi \psi^\dagger = (\phi \otimes \chi)(\phi \otimes \chi)^\dagger = (\phi^\dagger) \otimes (\chi^\dagger) .
\]

The set of separable states \( \mathcal{S}_1 \) is the smallest convex subset of \( \mathcal{D}_1 \) containing all the separable pure states. Since the separable pure states are extremal points of \( \mathcal{D}_1 \) containing \( \mathcal{S}_1 \), they are also extremal points of \( \mathcal{S}_1 \), and they are all the extremal points of \( \mathcal{S}_1 \). \( \mathcal{S}_1 \) is compact and defines a convex cone \( \mathcal{S} \subset \mathcal{D} \). The dimension of \( \mathcal{S}_1 \) is \( N^2 - 1 \), the same as the dimension of \( \mathcal{D}_1 \), hence every separable state may be written as a convex combination of \( N^2 \) or fewer pure product states \([38,39]\).

The fact that \( \mathcal{S} \) and \( \mathcal{D} \) have the same dimension \( N^2 \) is not quite as trivial as one might be tempted to think. It is a consequence of the fundamental fact that we use complex Hilbert spaces in quantum mechanics, as the following argument shows. In a quantum mechanics based on real Hilbert spaces every separable state would have to be symmetric under partial transposition, and the dimension of \( \mathcal{S} \) would be much smaller than the dimension of \( \mathcal{D} \). With complex Hilbert spaces, a generic real symmetric matrix which is a separable state is not symmetric under partial transposition, and the remarkable conclusion is that its representation as a convex combination of pure product states must necessarily involve complex product vectors. The basic reason that \( \mathcal{S} \) and \( \mathcal{D} \) have the same dimension is the relation \( \mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b \) between the real vector spaces \( \mathcal{H}, \mathcal{H}_a \) and \( \mathcal{H}_b \) of observables on \( \mathcal{H}, \mathcal{H}_a \) and \( \mathcal{H}_b \). We construct \( \mathcal{S} \) explicitly as a subset of \( \mathcal{H}_a \otimes \mathcal{H}_b \), in such a way that the dimension of \( \mathcal{S} \) is the full dimension of \( \mathcal{H}_a \otimes \mathcal{H}_b \).

We define the set of positive partial transpose states (PPT states) as \( \mathcal{P}_1 = \mathcal{D}_1 \cap \mathcal{D}_1^\dagger \). Partial transposition is an invertible linear operation preserving the convex structure of \( \mathcal{D}_1 \), hence \( \mathcal{P}_1 \)
is also a compact convex set defining a convex cone $\mathcal{P}$. We have that $\mathcal{S}_1 \subset \mathcal{P}_1 \subset \mathcal{D}_1$. The fact that every separable state has a positive partial transpose is obvious, and provides a simple and powerful test for separability, known as the Peres criterion [9]. In dimensions $2 \times 2$ and $2 \times 3$ the converse statement is also true, that every PPT state is separable [11]. The entanglement of PPT states is not distillable into entanglement of pure states, and it is believed that the entangled PPT states alone possess this special “bound” type of entanglement [19].

### 2.3 Dual cones, entanglement witnesses

The existence of entangled PPT states motivates the introduction of entanglement witnesses that may reveal their entanglement. We define the dual cone of $\mathcal{S}$ as

$$\mathcal{S}^o = \{ \Omega \in H \mid \text{Tr} \Omega \rho \geq 0 \forall \rho \in \mathcal{S} \}. \tag{5}$$

The members of $\mathcal{S}^o$ will be called here entanglement witnesses. The usual convention is that a witness is required to have at least one negative eigenvalue, but since our focus is on the geometry of $\mathcal{S}^o$ this restriction is not important to us here.

The definition of $\mathcal{S}^o$ as a dual cone implies that it is closed and convex. Since $\mathcal{S}$ is a closed convex cone the dual of $\mathcal{S}^o$ is $\mathcal{S}$ itself [11, 41] (the fact that $\mathcal{S}^{oo} = \mathcal{S}$ is given as an exercise in [41]). Thus, a witness having a negative expectation value in a state proves the state to be entangled, and given any entangled state there exists a witness having a negative expectation value in that state. This two-way implication makes entanglement witnesses powerful tools for detecting entanglement, both theoretically and experimentally [20, 26, 43–48].

From the experimental point of view the testimony of an entanglement witness is of a statistical nature. A positive or negative result of one single measurement of a witness gives little information about whether the state in question is separable or entangled. A positive or negative average over many measurements will give a more reliable answer, but some statistical uncertainty must always remain.

Since the extremal points of $\mathcal{S}_1$ are the pure product states, a matrix $\Omega \in H$ is a witness if and only if its expectation value is nonnegative in every pure product state. Furthermore, since the dimension of $\mathcal{S}$ is the full dimension of $H$, every witness $\Omega \neq 0$ has strictly positive expectation values in some pure product states. Since every product vector is a member of some basis of orthogonal product vectors, we conclude that every witness $\Omega \neq 0$ has $\text{Tr} \Omega > 0$ [12]. Accordingly the set $\mathcal{S}^o_1$ of normalized (unit trace) witnesses completely describes all of $\mathcal{S}^o$.

**Theorem 2.3.** $\mathcal{S}^o_1$ is a bounded set.

**Proof.** The maximally mixed state $\rho_0 = I/N$ is in $\mathcal{S}_1$. Define for $\theta > 0$ and $\Gamma \in H$ with $\text{Tr} \Gamma = 0$, $\text{Tr} \Gamma^2 = 1$,

$$f(\theta, \Gamma) = \min_{\rho \in \mathcal{S}_1} \text{Tr} \rho (\rho_0 + \theta \Gamma) = \frac{1}{N} + \theta \min_{\rho \in \mathcal{S}_1} \text{Tr} \rho \Gamma. \tag{6}$$

Since $\mathcal{S}_1$ is compact $f$ is well defined. Since $\text{Tr} \Gamma = 0$, we have $\Gamma \notin \mathcal{S}^o$ and the minimum of $\text{Tr} \rho \Gamma$ is strictly negative. Therefore, given any $\Gamma$ we can always find the $\theta(\Gamma)$ which makes $f(\theta, \Gamma) = 0$. Since $\Gamma$ lies in a compact set there exists a $\Gamma^*$ with $\theta^* = \theta(\Gamma^*) = \max_{\Gamma} \theta(\Gamma)$. This $\theta^*$ defines an $N^2 - 1$ dimensional Euclidean ball $\mathcal{B}_1$ centred at $\rho_0$ and containing $\mathcal{S}^o_1$. □
Note that the dual set $\mathcal{B}_1^\circ$ is an $N^2 - 1$ dimensional ball contained in $S_1$, also centred at $\rho_0$ [12].

From now on, when we talk about entanglement witnesses we will usually assume that they are normalized and lie in $S_1^\circ$. Since $S_1^\circ$ is a compact convex set it is completely described by its extremal points. The ultimate objective of the present work is to characterize these extremal witnesses.

The concept of dual cones applies of course also to the cone $\mathcal{D}$ of positive semidefinite matrices and the cone $\mathcal{P}$ of PPT matrices. The cone $\mathcal{D}$ is self-dual, $\mathcal{D}^\circ = \mathcal{D}$. Since $\mathcal{P} = \mathcal{D} \cap \mathcal{D}^P$, the dual cone $\mathcal{P}^\circ$ is the convex hull of $\mathcal{D} \cup \mathcal{D}^P$. Hence, the extremal points of $\mathcal{P}_1^\circ$ are the pure states $\psi \psi^\dagger$ and the partially transposed pure states $(\psi \psi^\dagger)^P$. These are also extremal in $S_1^\circ$ [14, 15, 24, 25]. A witness $\Omega \in \mathcal{P}^\circ$ is called decomposable, because it has the form

$$\Omega = \rho + \sigma^P$$

with $\rho, \sigma \in \mathcal{D}$. (7)

This terminology comes from the mathematical theory of positive maps [14]. Decomposable witnesses are in a sense trivial, and not very useful as witnesses, since they can not be used for detecting entangled PPT states.

Altogether, we have the following sequence of compact convex sets,

$$S_1 \subset \mathcal{P}_1 \subset \mathcal{D}_1 = \mathcal{D}_1^\circ \subset \mathcal{P}_1^\circ \subset S_1^\circ. \quad (8)$$

All these sets, with the exception of $\mathcal{D}_1$, are invariant under partial transposition. The sets $S_1$, $\mathcal{D}_1$, and $\mathcal{P}_1^\circ$ are very simply described in terms of their extremal points. The extremal points of $\mathcal{P}_1$ are not fully understood, though some progress has been made in this direction [18, 33–36]. The extremal points of $S_1^\circ$ are what we investigate here, they include the extremal points of $S_1$, $\mathcal{D}_1$, and $\mathcal{P}_1^\circ$.

A face of $\mathcal{D}_1$ is a complete set of density matrices on some subspace of $\mathcal{H}$ [10]. Faces of $S_1$ have recently been studied by Alfsen and Shultz [16, 49]. We also comment on faces of $S_1$ in Section 8. As we develop our results regarding extremal witnesses we will simultaneously obtain a classification of faces of $S_1^\circ$.

### 2.4 Positive maps

The study of the set of separable states through the dual set of entanglement witnesses was started by Michal, Pawel, and Ryszard Horodecki [11]. They pointed out the relation between witnesses and positive maps, and used known results from the mathematical theory of positive maps to throw light on the separability problem [14]. In particular, the fundamental result that there exist entangled PPT states is equivalent to the existence of nondecomposable positive maps.

We describe here briefly how entanglement witnesses are related to positive maps, but do not aim at developing the perspectives of positive maps in great detail. In Section 10 we return briefly to the use of positive maps for detecting entanglement.

We use a matrix $A \in H$ to define a real linear map $L_A: H_a \to H_b$ such that $Y = L_A X$ when

$$Y_{jl} = \sum_{i,k} A_{ij,kl} X_{ki}. \quad (9)$$

The correspondence $A \leftrightarrow L_A$ is a vector space isomorphism between $H$ and the space of real linear maps $H_a \to H_b$. A slightly different version of this isomorphism is more common in the literature, this is the Jamiołkowski isomorphism $A \leftrightarrow J_A$ by which $J_A X = L_A (X^\top)$ [50].
The transposed real linear map $L_A^\top : H_b \to H_a$ is defined such that $X = L_A^\top Y$ when
\[ X_{ik} = \sum_{j,l} A_{ij;kl} Y_{lj}. \tag{10} \]

It is the transpose of $L_A$ with respect to the natural scalar products $\langle U, V \rangle = \text{Tr} UV$ in $H_a$ and $H_b$. In fact, for any $X \in H_a$, $Y \in H_b$ we have
\[ \langle L_A X, Y \rangle = \text{Tr}(L_A X Y) = \sum_{i,j,k,l} A_{ij;kl} X_{ki} Y_{lj} = \text{Tr}(X (L_A^\top Y)) = \langle X, L_A^\top Y \rangle. \tag{11} \]

The maps $L_A$ and $L_A^\top$ act on one dimensional projection operators $\phi \phi^\dagger \in H_a$ and $\chi \chi^\dagger \in H_b$ according to
\[ L_A(\phi \phi^\dagger) = (\phi \otimes I_b)^\dagger A (\phi \otimes I_b), \]
\[ L_A^\top(\chi \chi^\dagger) = (I_a \otimes \chi)^\dagger A (I_a \otimes \chi). \tag{12} \]

Note that $\phi \otimes I_b$ is an $N \times N_b$ matrix such that $(\phi \otimes I_b) \chi = \phi \otimes \chi$, whereas $I_a \otimes \chi$ is an $N \times N_a$ matrix such that $(I_a \otimes \chi) \phi = \phi \otimes \chi$. It follows that
\[ \chi^\dagger (L_A(\phi \phi^\dagger)) \chi = \phi^\dagger (L_A^\top(\chi \chi^\dagger)) \phi = (\phi \otimes \chi)^\dagger A (\phi \otimes \chi). \tag{13} \]

If $\Omega$ is an entanglement witness then equation (13) implies that $L_\Omega$ is a positive linear map $H_a \to H_b$, mapping positive semidefinite matrices in $H_a$ to positive semidefinite matrices in $H_b$. Similarly, $L_\Omega^\top$ is a positive linear map $H_b \to H_a$. The correspondence $\Omega \leftrightarrow L_\Omega$ is a vector space isomorphism between the set of entanglement witnesses and the set of positive maps.

### 2.5 Biquadratic forms and optimization

The expectation value of an observable $A \in H$ in a pure product state $\psi \psi^\dagger$ with $\psi = \phi \otimes \chi$ is a biquadratic form
\[ f_A(\phi, \chi) = (\phi \otimes \chi)^\dagger A (\phi \otimes \chi). \tag{14} \]

The condition for $\Omega \in H$ to be an entanglement witness is that the biquadratic form $f_\Omega$ is positive semidefinite. Our approach here is to study witnesses through the associated biquadratic forms.

In the present work we study especially boundary witnesses, corresponding to biquadratic forms that are marginally positive. This leads naturally to an alternative definition of entanglement witnesses in terms of an optimization problem.

**Definition 2.2.** A matrix $A \in H$ is an entanglement witness if and only if the minimum value $p^\ast$ of the problem
\[ \text{minimize } f_A(\phi, \chi) = (\phi \otimes \chi)^\dagger A (\phi \otimes \chi), \quad \phi \in \mathcal{H}_a, \quad \chi \in \mathcal{H}_b, \]
subject to $\|\phi\| = \|\chi\| = 1$, \tag{15}
is nonnegative.
The normalization of $\phi$ and $\chi$ ensures that $p^* > -\infty$ when $A \notin S^\circ$, and that $p^* > 0$ for every $A$ in the interior of $S^\circ$. It is natural to use here the Hilbert–Schmidt norm introduced above, but in principle any norm would serve the same purpose.

The boundary $\partial S^\circ$ of $S^\circ$ consists of those $\Omega \in S^\circ$ for which there exists a separable state $\rho$ orthogonal to $\Omega$, i.e. with $\text{Tr} \Omega \rho = 0$. In terms of problem (15), $A \in \partial S^\circ$ if and only if $p^* = 0$. Since $S^\circ = S$ we can similarly understand the boundary of $S$ as the set of separable states orthogonal to some witness. We will return to this duality between the boundaries of $S$ and $S^\circ$ in Section 8.

2.6 Equivalence under SL $\otimes$ SL transformations

It is very useful to observe that all the main concepts discussed in the present article are invariant under what we call SL $\otimes$ SL transformations, in which a matrix $A$ is transformed into $VAV^\dagger$ with an invertible product matrix $V = V_a \otimes V_b$.

For example, since such a transformation is linear in $A$, it preserves convex combinations, extremal points, and in general all the convexity properties of different sets. It preserves the positivity of matrices, the tensor product structure of vectors and matrices, the number of zeros of witnesses, and in general all properties related to entanglement, except that it may increase or decrease entanglement as measured quantitatively if either $V_a$ or $V_b$ is not unitary.

Thus, for our purposes it is useful to consider two density matrices or two entanglement witnesses to be equivalent if they are related by an SL $\otimes$ SL transformation. This sorting into equivalence classes helps to reduce the problem of understanding and classifying entangled states and entanglement witnesses.

3 Secondary constraints at zeros of witnesses

By definition, a witness $\Omega$ satisfies the following infinite set of inequalities, all linear in $\Omega$,

$$f_\Omega(\phi, \chi) \geq 0 \quad \text{with} \quad \phi \in \mathcal{H}_a, \quad \chi \in \mathcal{H}_b, \quad \|\phi\| = \|\chi\| = 1.$$  \hfill (16)

These constraints on $\Omega$, represented here as a biquadratic form $f_\Omega$, are the primary constraints defining the set $S^\circ_1$, apart from the trivial linear constraint $\text{Tr} \Omega = 1$.

If $\Omega$ is situated on the boundary of $S^\circ_1$ it means that at least one of these primary inequalities is an equality. We will call the pair $(\phi_0, \chi_0)$ a zero of $\Omega$ if $f_\Omega(\phi_0, \chi_0) = 0$. We count $(a\phi_0, b\chi_0)$ with $a, b \in \mathbb{C}$ as the same zero. The primary constraints (16) with $(\phi, \chi)$ close to the zero $(\phi_0, \chi_0)$ lead to rather stringent constraints on $\Omega$, which we introduce as secondary constraints to be imposed at the zero. These secondary constraints are both equalities and inequalities, and they are linear in $\Omega$, like the primary constraints from which they are derived.

Though purely deductive, the exposition in this section is new, to our knowledge, although the basic secondary equality constraints have earlier been developed (Lemma A1 of [26]). See Appendix A. In the next section we apply all the secondary constraints to the problem of constructing and classifying extremal witnesses.

3.1 Positivity constraints on polynomials

A model example may illustrate how we treat constraints. Let $f(t)$ be a real polynomial in one real variable $t$, of degree four and with a strictly positive quartic term, satisfying the primary constraints $f(t) \geq 0$ for all $t$. These are constraints on the coefficients of the polynomial. The
equation \( f(t) = 0 \) can have zero, one or two real roots for \( t \). Assume that \( f(t_0) = 0 \). Because this is a minimum, we must have \( f'(t_0) = 0 \) and \( f''(t_0) \geq 0 \). In the limiting case \( f''(t_0) = 0 \) we must have also \( f^{(3)}(t_0) = 0 \).

Thus, if \( f(t_0) = 0 \) we get secondary constraints \( f'(t_0) = 0 \), and either \( f''(t_0) > 0 \) or \( f''(t_0) = 0, f^{(3)}(t_0) = 0 \). If there is a second zero \( t_1 \), similar secondary constraints must hold there. It should be clear that we may replace the infinite set of primary constraints \( f(t) \geq 0 \) for every \( t \) by the finite set of secondary constraints at the zeros \( t_0 \) and \( t_1 \).

Because the zeros of a witness \( \Omega \) are roots of a polynomial equation in several variables, they have the following property.

**Theorem 3.1.** The set of zeros of a witness consists of at most a finite number of components, where each component is either an isolated point or a continuous connected surface.

**Proof.** Choose \((\phi_2, \chi_2)\) such that \( f_\Omega(\phi_2, \chi_2) > 0 \), and define \( f(t) = f_\Omega(\phi_1 + t\phi_2, \chi_1 + t\chi_2) \). For given \((\phi_1, \chi_1)\) and \((\phi_2, \chi_2)\) this is a nonnegative polynomial in the real variable \( t \) of degree four, hence it has zero, one or two real roots for \( t \). By varying \((\phi_1, \chi_1)\) we reach all the zeros of \( \Omega \). The zeros of \( f(t) \) will move continuously when we vary \((\phi_1, \chi_1)\), except that they may appear or disappear. This construction should result in a set of zeros as described in the theorem. \( \square \)

Now let \((\phi_0, \chi_0)\) be a zero of \( \Omega \), with \( \|\phi_0\| = \|\chi_0\| = 1 \). Since the constraints \((16)\) on the polynomial \( f_\Omega \) at \((\phi, \chi) = (\phi_0 + \xi, \chi_0 + \zeta)\) are actually independent of the normalization conditions \( \|\phi\| = \|\chi\| = 1 \), we choose to abandon these nonlinear normalization conditions (nonlinear in the Hilbert–Schmidt norm) and replace them by the linear constraints \( \phi_0^\dagger \xi = 0, \chi_0^\dagger \zeta = 0 \). Strictly speaking, even these orthogonality conditions are not essential, the important point is that we vary \( \phi \) and \( \chi \) in directions away from \( \phi_0 \) and \( \chi_0 \).

We find that some of the secondary constraints on \( f_\Omega \) are intrinsically real equations rather than complex equations, therefore we introduce real variables \( x \in \mathbb{R}^{2N_a - 2}, y \in \mathbb{R}^{2N_k - 2} \) and write \( \xi = J_0 x, \zeta = K_0 y \) with \( \phi_0^\dagger J_0 = 0, \chi_0^\dagger K_0 = 0 \). Our biquadratic form is then a real inhomogeneous polynomial quadratic in \( x \) and quadratic in \( y \),

\[
\begin{align*}
f(x, y) &= f_\Omega(\phi, \chi) = ((\phi_0 + \xi) \otimes (\chi_0 + \zeta))^\dagger \Omega ((\phi_0 + \xi) \otimes (\chi_0 + \zeta)). \quad (17)
\end{align*}
\]

The linear term of the polynomial is

\[
egin{align*}
f_1(x, y) &= 2 \text{Re}((\xi \otimes \chi_0)^\dagger \Omega (\phi_0 \otimes \chi_0) + (\phi_0 \otimes \zeta)^\dagger \Omega (\phi_0 \otimes \chi_0)) \\
&= x^\top D_x f(0, 0) + y^\top D_y f(0, 0), \quad (18)
\end{align*}
\]

in terms of the gradient

\[
egin{align*}
D_x f(0, 0) &= 2 \text{Re}(J_0 \otimes \chi_0)^\dagger \Omega (\phi_0 \otimes \chi_0), \\
D_y f(0, 0) &= 2 \text{Re}(\phi_0 \otimes K_0)^\dagger \Omega (\phi_0 \otimes \chi_0). \quad (19)
\end{align*}
\]

The quadratic term is

\[
egin{align*}
f_2(x, y) &= (\xi \otimes \chi_0)^\dagger \Omega (\xi \otimes \chi_0) + (\phi_0 \otimes \zeta)^\dagger \Omega (\phi_0 \otimes \zeta) \\
&+ 2 \text{Re}((\phi_0 \otimes \zeta)^\dagger \Omega (\xi \otimes \chi_0) + (\phi_0 \otimes \chi_0)^\dagger \Omega (\xi \otimes \zeta)) \\
&= z^\top G_\Omega z, \quad (20)
\end{align*}
\]
where \( z^T = (x^T, y^T) \), and \( 2G_\Omega = D^2 f(0, 0) \) is the second derivative, or Hessian, matrix, which is real and symmetric,

\[
G_\Omega = \text{Re} \begin{bmatrix} g_{xx} & g_{yx}^T \\ g_{yx} & g_{yy} \end{bmatrix},
\]

\[
g_{xx} = (J_0 \otimes \chi_0)^\dagger \Omega (J_0 \otimes \chi_0),
\]

\[
g_{yy} = (\phi_0 \otimes K_0)^\dagger \Omega (\phi_0 \otimes K_0),
\]

\[
g_{yx} = (\phi_0 \otimes K_0)^\dagger \Omega (J_0 \otimes \chi_0) + (\phi_0 \otimes K_0)^\dagger \Omega^P (J_0 \otimes \chi_0^*).
\]

The cubic term is like the linear term but with \( \phi_0 \leftrightarrow \xi \) and \( \chi_0 \leftrightarrow \zeta \),

\[
f_3(x, y) = 2\text{Re}((\phi_0 \otimes \zeta)^\dagger \Omega (\xi \otimes \zeta) + (\xi \otimes \chi_0)^\dagger \Omega (\xi \otimes \zeta)).
\]

The quartic term is simply

\[
f_4(x, y) = f_\Omega(\xi, \zeta) = (\xi \otimes \zeta)^\dagger \Omega (\xi \otimes \zeta).
\]

The fact that the constant term of the polynomial vanishes, \( f(0, 0) = 0 \), is one real linear constraint on \( \Omega \),

\[
T_0 : H \to \mathbb{R}, \quad T_0 \Omega = (\phi_0 \otimes \chi_0)^\dagger \Omega (\phi_0 \otimes \chi_0) = 0.
\]

Because \( (x, y) = (0, 0) \) is a minimum of the polynomial the linear term must also vanish identically, and this results in another linear system of constraints,

\[
T_1 : H \to \mathbb{R}^{2(N_a + N_b - 2)}, \quad T_1 \Omega = \begin{bmatrix} D_x f(0, 0) \\ D_y f(0, 0) \end{bmatrix} = 0.
\]

Note that the equality constraints \( T_0 \) and \( T_1 \) are the same for every witness with the zero \((\phi_0, \chi_0)\), they are uniquely defined by the zero alone. The total number of constraints in \( T_0 \) and \( T_1 \) is

\[
M_2 = 2(N_a + N_b) - 3.
\]

All of these \( M_2 \) constraints are linearly independent. They are given an explicitly real representation in Appendix A.

It is worth noting that the vanishing of the constant and linear terms of the polynomial \( f(x, y) \) is equivalent to the conditions that

\[
(\phi \otimes \chi_0)^\dagger \Omega (\phi_0 \otimes \chi_0) = 0 \quad \forall \phi \in \mathcal{H}_a,
\]

\[
(\phi_0 \otimes \chi)^\dagger \Omega (\phi_0 \otimes \chi_0) = 0 \quad \forall \chi \in \mathcal{H}_b.
\]

Hence the \( 2(N_a + N_b) - 3 \) real constraints \( T_0 \Omega = 0 \) and \( T_1 \Omega = 0 \) may be expressed more simply as the following set of \( N_a + N_b \) complex constraints, equivalent to \( 2(N_a + N_b) \) real constraints that are then not completely independent,

\[
L_\Omega^\dagger (\chi_0 \chi_0) \phi_0 = (I_a \otimes \chi_0)^\dagger \Omega (\phi_0 \otimes \chi_0) = 0,
\]

\[
L_\Omega (\phi_0 \phi_0^\dagger) \chi_0 = (\phi_0 \otimes I_b)^\dagger \Omega (\phi_0 \otimes \chi_0) = 0.
\]

The quadratic term of the polynomial has to be nonnegative, again because \( (x, y) = (0, 0) \) is a minimum. The inequalities

\[
z^T G_\Omega z \geq 0 \quad \forall z \in \mathbb{R}^{2(N_a + N_b - 2)}
\]
are secondary inequality constraints, linear in $\Omega$, equivalent to the nonlinear constraints that all the eigenvalues of the Hessian matrix $G\Omega$ must be nonnegative.

There are now two alternatives. If the inequalities (29) hold with strict inequality for all $z \neq 0$, in other words, if all the eigenvalues of the Hessian are strictly positive, then we call $(\phi_0, \chi_0)$ a quadratic zero. In this case $T_0$ and $T_1$ are the only equality constraints placed on $\Omega$ by the existence of the zero $(\phi_0, \chi_0)$. We can immediately state the following important result.

**Theorem 3.2.** A quadratic zero is isolated: there is a finite distance to the next zero. Hence, a witness can have at most a finite number of quadratic zeros.

### 3.2 Hessian zeros

The second alternative is that the Hessian has $K$ zero eigenvalues with $K \geq 1$. We will call $z \neq 0$ a Hessian zero at the zero $(\phi_0, \chi_0)$ if $G\Omega z = 0$. It is then a real linear combination

$$z = \sum_{i=1}^{K} a_i z_i$$

of basis vectors $z_i \in \text{Ker} G\Omega$. The $K$ linearly independent eigenvectors $z_i$ define the following system of linear constraints on $\Omega$,

$$T_2: H \to \mathbb{R}^{2K(N_a+N_b-2)}, \quad (T_2 \Omega)_i = G\Omega z_i = 0, \quad i = 1, \ldots, K.$$  (31)

These constraints ensure that $G\Omega z = 0$ and hence $f_2(x,y) = z^T G\Omega z = 0$. The vanishing of the quadratic term of the polynomial implies that the cubic term must vanish as well. We therefore call $(\phi_0, \chi_0)$ a quartic zero, and the direction $z$ at $(\phi_0, \chi_0)$ a quartic direction. The vanishing cubic term is

$$f_3(x,y) = 2 \sum_{l,m,n} a_la_ma_n \text{Re}((\phi_0 \otimes \zeta_l)^\dagger \Omega(\xi_m \otimes \zeta_n) + (\xi_l \otimes \chi_0)^\dagger \Omega(\xi_m \otimes \zeta_n)) = 0,$$  (32)

where $\xi_i = J_0 x_i$ and $\zeta_i = K_0 y_i$. Since the product $a_la_ma_n$ is completely symmetric in the indices $l, m, n$ we should symmetrize the expression it multiplies. All the different properly symmetrized expressions must vanish. In this way we obtain a linear system

$$(T_3 \Omega)_{lmn} = 0 \quad \text{with} \quad 1 \leq l \leq m \leq n \leq K.$$  (33)

The number of equations is the binomial coefficient $\binom{K+2}{3}$, but it is likely that these constraints on $\Omega$ will in general not be independent.

The total number of constraints in $T_2$ and $T_3$ is therefore

$$M_4(K) = 2K(N_a + N_b - 2) + \binom{K+2}{3}. $$  (34)

Note that $M_4(1) = M_2 = 2(N_a + N_b) - 3$. Since the constraints in $T_2$ and $T_3$ address other terms in the polynomial than those in $T_0$ and $T_1$, the two sets of constraints should be independent from each other. Furthermore, in the case $K = 1$, all $M_4(1)$ equations in the total system $T_2, T_3$ should be linearly independent. In the case of $K > 1$ we expect overlapping constraints.
3.3 Summary of constraints

Let $\Omega$ be a witness, and let $Z$ be the complete set of zeros of $\Omega$, with $Z' \subseteq Z$ as the subset of quartic zeros. Each zero in $Z$ defines zeroth and first order equality constraints $T_0$ and $T_1$. The combination of a set of constraints is the direct sum. Thus we define $U_0$ as the direct sum of the constraints $T_0$ over all the zeros in $Z$, and similarly $U_1$ as the direct sum of the constraints $T_1$. We define $U_{01} = U_0 \oplus U_1$. Each zero in $Z'$ introduces additional second and third order constraints $T_2$ and $T_3$. We denote the direct sums of these by $U_2$ and $U_3$, respectively, and we define $U_{23} = U_2 \oplus U_3$. Denote by $U_\Omega$ the full system of constraints on $\Omega$, $U_\Omega = U_{01} \oplus U_{23}$.

It is an important observation that all the constraints are completely determined by the zeros and Hessian zeros of $\Omega$. Thus they depend only indirectly on $\Omega$. In particular, $U_{01}$ depends only on $Z$, whereas $U_{23}$ depends on $Z'$ and on the kernel of the Hessian at each quartic zero.

A boundary witness with only quadratic zeros will be called here a quadratic boundary witness, or simply a quadratic witness, since we are talking most of the time about boundary witnesses. A boundary witness with at least one quartic zero will be called a quartic witness. Note that if $\Omega$ is quadratic then $Z'$ is empty so $U_{01} = U_{01}$. This classification of boundary witnesses as quadratic and quartic is fundamental, since the two classes have rather different properties. The quadratic witnesses turn up in much greater numbers in random searches, and are also simpler to understand theoretically.

4 Extremal witnesses

In this section we apply the constraints developed in the previous section to study extremal witnesses. We approach the problem through the basic definition that a nonextremal witness is one which can be written as a convex combination of other witnesses. In the language of convex sets it is an interior point of a face of $S^\circ_1$ of dimension one or higher.

In Subsection 4.1 we characterize the extremal witnesses in terms of their zeros. In Subsections 4.2 and 4.3 we characterize them in terms of the constraints related to their zeros. and present a search algorithm for finding them numerically. The geometrical interpretation of this algorithm is that we start from a given witness, reconstruct the unique face of $S^\circ_1$ of which it is an interior point, go to the boundary of this face, and repeat the process. In Subsection 4.4 we discuss the expected number of zeros of extremal witnesses.

The theorems 4.3 and 4.5 give necessary and sufficient conditions for a witness to be extremal, and they are main results of our work.

4.1 Zeros of witnesses, convexity and extremality

Let $\Omega$ be a convex combination of two different witnesses $\Lambda$ and $\Sigma$,

$$\Omega = (1 - p) \Lambda + p \Sigma,$$

with $0 < p < 1$. Then the corresponding biquadratic form is a convex combination

$$f_{\Omega}(\phi, \chi) = (1 - p) f_\Lambda(\phi, \chi) + p f_\Sigma(\phi, \chi),$$

and the Hessian matrix at any zero $(\phi_0, \chi_0)$ of $\Omega$ is also a convex combination

$$G_{\Omega} = (1 - p) G_\Lambda + p G_\Sigma.$$
The facts that the biquadratic form of an entanglement witness is positive semidefinite, and that the Hessian matrix at any zero of a witness is also positive semidefinite, imply the following result.

**Theorem 4.1.** If \( \Omega \) is a convex combination of two witnesses \( \Lambda \) and \( \Sigma \), as above, then \( (\phi_0, \chi_0) \) is a zero of \( \Omega \) if and only if it is a zero of both \( \Lambda \) and \( \Sigma \).

Similarly, \( z \) is a Hessian zero of \( \Omega \) at the zero \( (\phi_0, \chi_0) \) if and only if it is a Hessian zero at \( (\phi_0, \chi_0) \) of both \( \Lambda \) and \( \Sigma \).

Thus, all witnesses in the interior of the line segment between \( \Lambda \) and \( \Sigma \) have exactly the same zeros and Hessian zeros.

Assume further that \( \Lambda \) and \( \Sigma \) are extremal points of the intersection of the straight line with \( S_1^o \), so that \( \Omega \not\in S_1^o \) when \( p < 0 \) and when \( p > 1 \). To be specific, consider the case \( p > 1 \). We want to show that \( \Sigma \) has at least one zero or Hessian zero in addition to the zeros and Hessian zeros of the witnesses in the interior of the line segment.

By assumption, the set of negative points

\[
X_-(p) = \{ (\phi, \chi) \mid f_\Omega(\phi, \chi) < 0 \}
\]

is nonempty for \( p > 1 \). Clearly \( X_-(p) \subset X_-(q) \) for \( 1 < p < q \), since \( X_-(p) \) is empty for \( 0 \leq p \leq 1 \), and \( f_\Omega(\phi, \chi) \) is a linear function of \( p \) for fixed \( (\phi, \chi) \) as given by equation (36). The closure \( \overline{X}_-(p) \) is a compact set when we normalize so that \( \|\phi\| = \|\chi\| = 1 \). It follows that the limit of \( \overline{X}_-(p) \) as \( p \to 1^+ \) is a nonempty set \( X_0 \) of zeros of the witness \( \Sigma \),

\[
X_0 = \bigcap_{p > 1} \overline{X}_-(p).
\]

Every zero \( (\phi_0, \chi_0) \in X_0 \) is of the kind we are looking for. If it is not a zero of \( \Omega \) for \( p < 1 \), then it is a new zero of \( \Sigma \) as compared to the zeros of the witnesses in the interior of the line segment. If it is a zero of \( \Omega \) for \( p < 1 \), then \( \Sigma \) has at least one Hessian zero at \( (\phi_0, \chi_0) \) which is not a Hessian zero at \( (\phi_0, \chi_0) \) of the witnesses in the interior of the line segment.

To prove the last statement, assume that \( (\phi_0, \chi_0) \in X_0 \) is a zero of \( \Omega \) for \( 0 < p < 1 \). Then it is a zero of \( \Omega \) for any \( p \), again because \( f_\Omega(\phi, \chi) \) is a linear function of \( p \). Similarly, if \( z \) is a Hessian zero of \( \Omega \) at \( (\phi_0, \chi_0) \) for \( 0 < p < 1 \), it is a Hessian zero of \( \Omega \) at \( (\phi_0, \chi_0) \) for any \( p \).

From the assumption that \( (\phi_0, \chi_0) \in X_0 \) follows that \( f_\Omega(\phi, \chi) \) for any \( p > 1 \) takes negative values for some \( (\phi, \chi) \) arbitrarily close to \( (\phi_0, \chi_0) \). The only way this may happen is that for \( p > 1 \) the second derivative \( z^T G_\Omega z \) is negative in some direction \( z \), meaning that \( G_\Omega \) for \( p > 1 \) has one or more negative eigenvalues \( \lambda_i(p) \), with eigenvectors \( z_i(p) \) that are orthogonal to each other and orthogonal to the \( p \) independent part of \( \text{Ker} G_\Omega \).

In the limit \( p \to 1^+ \) the negative eigenvalues \( \lambda_i(p) \) of \( G_\Omega \) go to zero, and the corresponding eigenvectors \( z_i(p) \) go to eigenvectors \( z_i(1) \) of \( G_\Sigma \) with zero eigenvalues. These eigenvectors are then Hessian zeros of \( \Sigma \) at \( (\phi_0, \chi_0) \) that are not Hessian zeros of \( \Omega \) for \( 0 < p < 1 \).

We summarize the present discussion as follows.

**Theorem 4.2.** If a line segment in \( S_1^o \) with end points \( \Lambda \) and \( \Sigma \) can not be prolonged within \( S_1^o \) in either direction, then \( \Sigma \) has the same zeros and Hessian zeros as the interior points of the line segment, and at least one additional zero or Hessian zero.

The same holds for \( \Lambda \), with additional zeros and Hessian zeros that are different from those of \( \Sigma \).
These theorems lead to the following extremality criterion for witnesses.

**Theorem 4.3.** A witness $\Omega$ is extremal if and only if no witness $\Lambda \neq \Omega$ has a set of zeros and Hessian zeros including the zeros and Hessian zeros of $\Omega$.

An equivalent condition is that no witness $\Lambda \neq \Omega$ satisfies the constraints $U_\Omega \Lambda = 0$.

*Proof.* The “if” part follows directly from Theorem 4.1.

To prove the “only if” part, assume that the set of zeros and Hessian zeros of some witness $\Lambda \neq \Omega$ include the zeros and Hessian zeros of $\Omega$. Then by Theorem 4.1 the interior points of the line segment with $\Lambda$ and $\Omega$ as end points have exactly the same zeros and Hessian zeros as $\Omega$. By Theorem 4.2 this line segment can be prolonged within $S^0$ so that it gets $\Omega$ as an interior point. Hence $\Omega$ is not extremal. \qed

### 4.2 How to search for extremal witnesses

Once the zeros and Hessian zeros of a witness $\Omega$ are known, it is a simple computational task to find a finite perturbation of $\Omega$ within the unique face of $S^0$ where $\Omega$ is an interior point. The most general direction for such a perturbation is a traceless $\Gamma \in \text{Ker } U_\Omega$. Note that we only need to find some $\Gamma' \in \text{Ker } U_\Omega$ not proportional to $\Omega$, then $\Gamma = \Gamma' - (\text{Tr } \Gamma') \Omega$ is nonzero and traceless and lies in $\text{Ker } U_\Omega$.

**Theorem 4.4.** Let $\Omega$ be a witness, and let $\Gamma \in H$, $\Gamma \neq 0$, $\text{Tr } \Gamma = 0$. Then $\Lambda = \Omega + t \Gamma$ is a witness for all $t$ in some interval $[t_1, t_2]$, with $t_1 < 0 < t_2$, if and only if $\Gamma \in \text{Ker } U_\Omega$.

The maximal value of $t_2$ is the value of $t$ where $\Lambda$ acquires a new zero or Hessian zero. The minimal value of $t_1$ is determined in the same way.

*Proof.* To prove the “only if” part, assume that $\Lambda = \Omega + t \Gamma$ is a witness for $t_1 \leq t \leq t_2$. Then by Theorem 4.1, $\Lambda$ has the same zeros and Hessian zeros as $\Omega$ for $t_1 < t < t_2$. Since the constraints $U_\Omega$ depend only on the zeros and Hessian zeros of $\Omega$, we conclude that $U_\Omega \Lambda = 0$ for $t_1 < t < t_2$, and hence $U_\Omega \Gamma = 0$.

To prove the “if” part, assume that $U_\Omega \Gamma = 0$. Since $U_\Omega \Omega = 0$, it follows that $U_\Omega \Lambda = 0$ for any value of $t$. Consider the set of negative points,

$$X_-(t) = \{ (\phi, \chi) \mid f_\Lambda(\phi, \chi) < 0 \}.$$  \hspace{1cm} (40)

We want to argue that $X_-(t)$ must be empty for $t$ in some interval $[t_1, t_2]$ with $t_1 < 0 < t_2$.

In fact, since $S^0$ is a compact set, there must exist some $t_2 \geq 0$ such that $X_-(t)$ is empty for $0 \leq t < t_2$ and nonempty for $t > t_2$. Then the limit of $X_-(t)$ as $t \to t_2+$ is a nonempty set $X_0$ of zeros of $\Lambda_2 = \Omega + t_2 \Gamma$. A similar reasoning as the one leading to Theorem 4.2 now leads us to the conclusion that $\Lambda_2$ must have at least one zero or Hessian zero which is not a zero or Hessian zero of $\Omega$. This proves that $\Lambda_2 \neq \Omega$ and $t_2 > 0$.

By a similar argument we deduce the existence of a lower limit $t_1 < 0$. \qed

Figure 1 shows a model for how a new isolated quadratic zero of $\Lambda$ appears, or how an existing quadratic zero turns into a quartic zero, as the parameter $t$ increases in the function

$$f_t(u) = f_{\Omega + t \Gamma}(\phi + u \phi', \chi + u \chi').$$  \hspace{1cm} (41)

The next theorem is an immediate corollary. It is a slightly stronger version of Theorem 4.3. It is interesting for the theoretical understanding, and together with Theorem 4.4 it is directly useful for numerical calculations.
Figure 1: Models for how the positivity limit is reached. Left: a new local minimum appears, turning into a zero and then a negative minimum. The model function plotted for five different values of $t$ is $f_t(u) = u^2((u - 1)^2 + 1 - t)$, depending on a parameter $t$ with the critical value $t_c = 1$. Right: a quadratic zero turns into a quartic zero, and then new negative minima branch off. The model function is $f_t(u) = u^2(u^2 + 1 - t)$, again with the critical parameter value $t_c = 1$.

**Theorem 4.5.** A witness $\Omega$ is extremal if and only if $\text{Ker} \mathbf{U}_\Omega$ is one dimensional (spanned by $\Omega$).

Thus, once the zeros and Hessian zeros of the witness $\Omega$ are known we test for extremality by computing the dimension of $\text{Ker} \mathbf{U}_\Omega$, for example by a singular value decomposition of $\mathbf{U}_\Omega$. This allows for a simple numerical implementation of the extremality criterion.

These theorems motivate Algorithm 1, a search algorithm for finding extremal witnesses. Obviously, any extremal witness might be reached by this algorithm already in the first iteration, starting for example from the maximally mixed state. The search is guaranteed to converge to an extremal witness in a finite number of iterations, since the number of possible search directions is reduced in each iteration.

**Algorithm 1** Find an extremal witness

**Require:** an initial witness $\Omega$, e.g. the maximally mixed state

1: locate all zeros of $\Omega$, if any, and construct $\mathbf{U}_\Omega$
2: while $\dim \text{Ker} \mathbf{U}_\Omega > 1$ do
3: choose a $\Gamma \in \text{Ker} \mathbf{U}_\Omega$
4: if $\text{Tr} \Gamma \neq 0$ redefine $\Gamma \leftarrow \Gamma - (\text{Tr} \Gamma) \Omega$
5: find $t_c$ as the maximal $t$ such that $\Omega + t \Gamma$ is a witness
6: redefine $\Omega \leftarrow \Omega + t_c \Gamma$
7: locate all zeros of $\Omega$ and construct $\mathbf{U}_\Omega$
8: end while
9: return $\Omega$
4.3 Faces of the set $S^0_1$ of normalized witnesses

Theorem 4.4 has the following geometrical meaning. Define

$$F_\Omega = (\text{Ker } U_\Omega) \cap S^0_1.$$  \hfill (42)

Equivalently, define $F_\Omega$ as the set of all witnesses of the form $\Omega + t\Gamma$ with $\Gamma \in \text{Ker } U_\Omega$ and $\text{Tr } \Gamma = 0$. If $\Omega$ is extremal in $S^0_1$ then $F_\Omega$ consists of the single point $\Omega$. Otherwise, $F_\Omega$ is the unique face of $S^0_1$ having $\Omega$ as an interior point.

Thus, Algorithm 1 produces a decreasing sequence of faces of $S^0_1$, $F_1 \supset F_2 \supset \ldots \supset F_n$, where every face $F_j$ is a face of every $F_i$ with $i < j$, and the extremal point found is an extremal point of all these faces.

The theorems in Subsection 4.1 imply that every face $F$ of $S^0_1$ is uniquely characterized by a set of zeros and Hessian zeros that is the complete set of zeros and Hessian zeros of every witness in the interior of $F$. Every boundary point of $F$ is a witness having the zeros and Hessian zeros characteristic of the interior points, plus at least one more zero or Hessian zero. In general, the boundary of $S^0_1$ is a hierarchy of faces, faces of faces, faces of faces of faces, and so on. The number of zeros and Hessian zeros increases each time we step from one face onto a face of the face, and the descent through the hierarchy from one face to the next always ends in an extremal witness.

4.4 Zeros of extremal witnesses

A natural question regards the number of zeros a witness must have in order to be extremal. We provide two lower bounds for quadratic witnesses, one obtained by comparison with a pure state as a witness and the other by counting constraints. Similar bounds for quartic witnesses are not easy to obtain.

The first of these bounds reveals a “double spanning” property of zeros of quadratic extremal witnesses. We define the partial conjugate of $(\phi, \chi)$ as $(\phi, \chi^*)$.

**Theorem 4.6.** The zeros of a quadratic extremal witness $\Omega$ span the Hilbert space. The partially conjugated zeros also span the Hilbert space.

**Proof.** Assume that the zeros span less than the whole Hilbert space, so that there exists a vector $\psi$ orthogonal to all the zeros. Then the projection $P = \psi\psi^\dagger$ is a witness with a set of zeros including all the zeros of $\Omega$. But $P$ has a continuum of zeros, all quartic, see Theorem 5.2. Hence $P \neq \Omega$ and $\Omega$ is not extremal, by Theorem 4.3.

The partial conjugates of the zeros of $\Omega$ span the Hilbert space because they are the zeros of the quadratic extremal witness $\Omega^p$.

This proof does not hold when $\Omega$ is a quartic witness, because $\Omega$ may then have Hessian zeros that are not Hessian zeros of $P$. A pure state $\psi\psi^\dagger$ as a quartic extremal witness is a counterexample, where the zeros do not span the Hilbert space, although the partially conjugated zeros may span the Hilbert space. The partial transpose $(\psi\psi^\dagger)^P$ is a counterexample of the opposite kind, where the zeros may span the Hilbert space but the partially conjugated zeros do not. Furthermore, even if neither the zeros nor the partially conjugated zeros span the Hilbert space, it is still possible for a quartic witness to be extremal, because a quartic zero leads to more constraints than a quadratic zero. In Subsection 6.3.2 we describe the numerical construction of an extremal quartic witness in dimension $3 \times 3$ with only 8 zeros, and with one Hessian zero at one of the zeros.
Counting constraints from quadratic zeros gives a different lower bound for the number of zeros of a quadratic extremal witness. There are $M_2 = 2(N_a + N_b) - 3$ constraints per quadratic zero. With $n$ quadratic zeros there are a total of $nM_2$ constraints, which in the generic case are linearly independent until $nM_2$ approaches $N^2 - 1$, the dimension of $S_1^2$. A lower bound on the number of zeros of a quadratic extremal witness is then given by

$$n_c = \text{ceil} \left( \frac{(N_a N_b)^2 - 1}{2(N_a + N_b) - 3} \right),$$

where ceil rounds upwards to the nearest integer.

In the special case $N_a = 2$ this formula gives the lower bound $n_c = N - 1$, which is weaker than the lower bound $N$ given by Theorem 4.6. When $N_a \geq 3$ and $N_b \geq 3$ the formula gives a lower bound $n_c \geq N$, consistent with Theorem 4.6.

Table 1 lists the numerically computed number of linearly independent constraints $m_{\text{ind}}$ arising from $n_c$ randomly chosen pairs $(\phi, \chi)$. In order to compute $m_{\text{ind}}$ we interpret each $(\phi, \chi)$ as a quadratic zero, build $U_{01}$ and do a singular value decomposition. The table shows that in many cases the number of independent constraints from a random set of product vectors is equal to the dimension of the real vector space $H$ of Hermitian matrices. In such a case there exists no biquadratic form which is positive semidefinite and has these zeros. We conclude that the zeros of a positive semidefinite biquadratic form have to satisfy some relations that reduce the number of independent constraints.

In the case $N_a = 2$ there is an intrinsic degeneracy with $n_c = N - 1$ random product vectors reducing the number of constraints by one. For example, in the $2 \times 4$ system the actual number of constraints from $n_c = 7$ random product vectors is 62 instead of $63 = n_c M_2$. This degeneracy implies that one extra zero is needed, thus saving Theorem 4.6. The proof of Theorem 4.6 indicates the origin of the degeneracy. With $N - 1$ zeros there exists a vector $\psi$ orthogonal to all the zeros and a vector $\eta$ orthogonal to all the partially conjugated zeros, and because $\psi\psi^\dagger$ and $(\eta\eta^\dagger)^P$ both lie in $\text{Ker } U_{01}$ we must have $\text{dim Ker } U_{01} \geq 2$. For other dimensions there is no similar degeneracy.

In $2 \times N_b$ and $3 \times 3$ systems, the minimum number of zeros of a quadratic extremal witness is exactly equal to the dimension $N = N_a N_b$ of the composite Hilbert space $H$. For the other dimensions, the minimum number of zeros to define a quadratic extremal witness is strictly larger than the dimension of $H$. This difference between $2 \times N_b$ and $3 \times 3$ systems on the one hand, and higher dimensional systems on the other hand, has important consequences discussed in Sections 8 and 9.

The $3 \times 4$ system is special in that the number of constraints from a generic set of $n_c = 13$ product vectors add up to exactly the number needed to define a unique $A \in H$ with $U_{01} A = 0$. This does not however imply that $A$ defined in this way from a random set of product vectors will be an extremal witness, in fact it will usually not be a witness, because it will have both positive and negative expectation values in product states.

A central question in general, well worth further attention, is how to choose a set of product vectors such that they may serve as the zeros of an extremal witness. According to Theorem 8.4, the zeros of a witness must define pure states lying on a face of the set $S$ of separable states. However, this statement leaves open the practical question of how to test numerically whether a set of pure product states lies on a face of $S$. 


| $N_a, N_b$ | $N^2$ | $M_2$ | $n_c$ | $m_{ind}$ |
|----------|-------|-------|-------|----------|
| 2,2      | 16    | 5     | 3     | 14       |
| 2,3      | 36    | 7     | 5     | 34       |
| 2,4      | 64    | 9     | 7     | 62       |
| 2,5      | 100   | 11    | 9     | 98       |
| 3,3      | 81    | 9     | 9     | 81       |
| 3,4      | 144   | 11    | 13    | 143      |
| 3,5      | 225   | 13    | 18    | 225      |
| 4,4      | 256   | 13    | 20    | 256      |
| 4,5      | 400   | 15    | 27    | 400      |
| 5,5      | 625   | 17    | 37    | 625      |

Table 1: Numbers related to quadratic zeros of witnesses in dimension $N = N_a N_b$. $M_2$ is the number of linearly independent constraints from each zero. $n_c$ is the estimated minimum number of zeros required for a quadratic witness to be extremal, assuming maximal independence of constraints. $m_{ind}$ is the actual number of independent constraints from $n_c$ random product vectors. Note that for $N_a = 2$ there is an intrinsic degeneracy causing the number of constraints from $n_c$ zeros to be $n_c M_2 - 1$, so the actual minimum number of zeros is $n_c + 1 = N$.

5 Decomposable witnesses

A decomposable witness is called so because it corresponds to a decomposable positive map, and because it has the form $\Omega = \rho + \sigma^P$ with $\rho, \sigma \in \mathcal{D}$, possibly $\rho = 0$ or $\sigma = 0$. Although the decomposable witnesses are useless for detecting entangled PPT states, they are useful in other ways, for example as stepping stones in some of our numerical methods for constructing extremal nondecomposable witnesses.

In this section we will summarize some basic properties of decomposable witnesses. This is a natural place to start when we want to understand entanglement witnesses in general. In particular, we are interested in the relation between a witness and its zeros.

Since the set $\mathcal{P}_1^0$ of decomposable witnesses is the convex hull of $\mathcal{D}_1$ and $\mathcal{D}_P^1$, an extremal point of $\mathcal{P}_1^0$ must be an extremal point of either $\mathcal{D}_1$ or $\mathcal{D}_P^1$. That is, it must be either a pure state $\psi \psi^\dagger$ or a partially conjugated pure state $(\psi \psi^\dagger)^P$, or both if $\psi$ is a product vector. In the present section we verify the results of [14, 24, 25] that witnesses of the forms $\psi \psi^\dagger$ and $(\psi \psi^\dagger)^P$ are extremal in $\mathcal{S}_1^o$. Since they are extremal in $\mathcal{S}_1^o$, they are also extremal in the subset $\mathcal{P}_1^0 \subset \mathcal{S}_1^o$. Thus they are precisely the extremal points of $\mathcal{P}_1^0$.

5.1 Zeros of a decomposable witness

The biquadratic form corresponding to the decomposable witness $\Omega = \rho + \sigma^P$ is

$$f_\Omega(\phi, \chi) = f_\rho(\phi, \chi) + f_\sigma(\phi, \chi^*) . \quad (44)$$

It is positive semidefinite because $f_\rho$ and $f_\sigma$ are positive semidefinite.

Assume now that $(\phi_0, \chi_0)$ is a zero of $\Omega$. The above decomposition of $f_\Omega$ shows that $(\phi_0, \chi_0)$ must be a zero of $\rho$, and the partial conjugate $(\phi_0, \chi_0^*)$ must be a zero of $\sigma$. But because $\rho, \sigma \in \mathcal{D}$ it follows that

$$\rho(\phi_0 \otimes \chi_0) = 0, \quad \sigma(\phi_0 \otimes \chi_0^*) = 0 . \quad (45)$$
This proves the following theorem.

**Theorem 5.1.** The zeros of a decomposable witness \( \Omega = \rho + \sigma^P \) span the Hilbert space only if \( \rho = 0 \). The partially conjugated zeros span the Hilbert space only if \( \sigma = 0 \).

Hence, by Theorem 4.6, a quadratic extremal witness is nondecomposable.

Note that if \( (\phi_0, \chi_0) \) is a zero of \( \Omega \) and \( \phi \otimes \chi \) is any product vector, then

\[
(\phi \otimes \chi_0)\sigma^P(\phi_0 \otimes \chi) = (\phi \otimes \chi^*)\sigma(\phi_0 \otimes \chi^*) = 0 \tag{46}
\]

and hence

\[
(\phi \otimes \chi_0)\Omega(\phi_0 \otimes \chi) = (\phi \otimes \chi_0)\rho(\phi_0 \otimes \chi) \tag{47}
\]

Similarly,

\[
(\phi \otimes \chi_0^*)\rho^P(\phi_0 \otimes \chi^*) = (\phi \otimes \chi_0^*)\rho(\phi_0 \otimes \chi_0) = 0 \tag{48}
\]

and hence

\[
(\phi \otimes \chi_0^*)\Omega^P(\phi_0 \otimes \chi^*) = (\phi \otimes \chi_0^*)\sigma(\phi_0 \otimes \chi^*) \tag{49}
\]

These equations may be useful for computing \( \rho \) and \( \sigma \) if \( \Omega \) is known but its decomposition \( \Omega = \rho + \sigma^P \) is unknown. We will return to this problem in Subsection 5.3.

### 5.2 Pure states and partially transposed pure states

Let \( P \) be a pure state, \( P = \psi \psi^\dagger \), and let \( Q \) be the partial transpose of a pure state, \( Q = (\eta \eta^\dagger)^P \), with \( \psi, \eta \in \mathcal{H} \). The corresponding positive maps \( L_P \) and \( L_Q \) are rank one preservers: they map matrices of rank one to matrices of rank one or zero, because

\[
L_P(\phi \phi^\dagger) = (\phi \otimes I_b)^\dagger P(\phi \otimes I_b) = \zeta \zeta^\dagger \quad \text{with} \quad \zeta = (\phi \otimes I_b)^\dagger \psi, \tag{50}
\]

and

\[
L_Q(\phi \phi^\dagger) = (\phi \otimes I_b)^\dagger Q(\phi \otimes I_b) = \zeta \zeta^\dagger \quad \text{with} \quad \zeta = (\phi^* \otimes I_b)^\dagger \eta^*. \tag{51}
\]

The corresponding biquadratic forms are positive semidefinite because they are absolute squares,

\[
f_P(\phi, \chi) = (\phi \otimes \chi)^\dagger P(\phi \otimes \chi) = |\psi^\dagger (\phi \otimes \chi)|^2, \tag{52}
\]

and

\[
f_Q(\phi, \chi) = (\phi \otimes \chi)^\dagger Q(\phi \otimes \chi) = (\phi \otimes \chi^*)^\dagger Q^P(\phi \otimes \chi^*) = |\eta^\dagger (\phi \otimes \chi^*)|^2. \tag{53}
\]

The zeros of \( P \) are the product vectors orthogonal to \( \psi \). A singular value decomposition (Schmidt decomposition) gives orthonormal bases \( \{u_i\} \) in \( \mathcal{H}_a \) and \( \{v_j\} \) in \( \mathcal{H}_b \) such that

\[
\psi = \sum_{i=1}^{m} c_i u_i \otimes v_i \quad \text{with all} \quad c_i > 0. \tag{54}
\]

Here \( m \) is the Schmidt number of \( \psi \), \( 1 \leq m \leq \min(N_a, N_b) \). The condition for a product vector

\[
\phi \otimes \chi = \sum_{i=1}^{N_a} \sum_{j=1}^{N_b} a_i b_j u_i \otimes v_j \tag{55}
\]
to be orthogonal to $\psi$ is that
\[ \sum_{i=1}^{m} c_i a_i b_i = 0. \] (56)

For any dimensions $N_a \geq 2$, $N_b \geq 2$ and any Schmidt number $m$ the set of zeros is continuous and connected. All the zeros are quartic, since quadratic zeros are isolated. The zeros do not span the whole Hilbert space, only the subspace orthogonal to $\psi$. However, the partially conjugated zeros span the Hilbert space, except when $\psi$ is a product vector, i.e. when $m = 1$. This almost completes the proof of the following theorem, what remains is to prove the extremality.

**Theorem 5.2.** A pure state as a witness has only quartic zeros, all in one continuous connected set, and it is extremal in $\mathcal{S}_0^\dagger$. The same is true for the partial transpose of a pure state.

**Proof.** We want to prove that $P$ is extremal, the proof for $Q$ is similar. We show that the only witness $\Omega$ satisfying the constraints $\mathbf{U}_P \Omega = 0$ is $\Omega = P$, from this we conclude that $P$ is extremal, according to Theorem 4.3.

Even though the zeros of $P$ are all quartic, they are so many that we need not use the secondary constraints coming from the quartic nature of the zeros. According to equation (28), the constraints $\mathbf{U}_P \Omega = 0$ include the constraints $\mathbf{L}_\Omega(\phi \phi^\dagger) \chi = 0$ for every zero $(\phi, \chi)$ of $P$. The zeros of $P$ are the solutions of the equation $\psi^\dagger(\phi \otimes \chi) = 0$. For every $\phi \in \mathcal{H}_a$ this is one linear equation for $\chi \in \mathcal{H}_b$, the solutions of which form a subspace of $\mathcal{H}_b$ of dimension either $N_b - 1$ or $N_b$. But this means that $\mathbf{L}_\Omega(\phi \phi^\dagger)$ has rank either one or zero, so that the positive map $\mathbf{L}_\Omega$ is a rank one preserver. Hence, either $\Omega = \omega \omega^\dagger$ or $\Omega = (\tilde{\omega} \tilde{\omega}^\dagger)^P$ for some $\omega, \tilde{\omega} \in \mathcal{H}$ [24].

In the first case, $\Omega = \omega \omega^\dagger$, we must have $\omega^\dagger(\phi \otimes \chi) = 0$ for every $(\phi, \chi)$ such that $\psi^\dagger(\phi \otimes \chi) = 0$. But then $\omega$ must be proportional to $\psi$, and $\Omega = P$.

In the second case, $\Omega = (\tilde{\omega} \tilde{\omega}^\dagger)^P$, we must have $\tilde{\omega}^\dagger(\phi \otimes \chi^*) = 0$ for every $(\phi, \chi)$ such that $\psi^\dagger(\phi \otimes \chi) = 0$. This is possible, but only if $\psi$ and $\tilde{\omega}$ are product vectors, with $\tilde{\omega}$ the partial conjugate of $\psi$. Then we again have $\Omega = P$. $\square$

The fact that every zero $(\phi_0, \chi_0)$ of $P$ is quartic can also be seen directly from equation (20). With $\Omega = P = \psi \psi^\dagger$ and $\psi^\dagger(\phi_0 \otimes \chi_0) = 0$ equation (20) takes the form
\[ z^\dagger G_\Omega z = f_2(x, y) = |\psi^\dagger(\xi \otimes \chi_0 + \phi_0 \otimes \zeta)|^2. \] (57)

Thus, $z^\dagger G_\Omega z = 0$ unless the vector $\xi \otimes \chi_0 + \phi_0 \otimes \zeta \in \mathcal{H}$ has a component along $\psi$. This means that the Hessian matrix $G_\Omega$ at the zero $(\phi_0, \chi_0)$ has rank at most two.

### 5.3 Decomposing a decomposable witness

If we want to prove that a given witness $\Omega$ is decomposable, the definitive solution is of course to decompose it as $\Omega = \rho + \sigma^P$ with $\rho, \sigma \in \mathcal{D}$. We want to discuss here methods for doing this, based on a knowledge of zeros of $\Omega$. Unfortunately, the present discussion does not lead to a complete solution of the problem.

Assume that we know a finite set of $k$ zeros of $\Omega$, $Z = \{ \phi_i \otimes \chi_i \}$, with partial conjugates $\tilde{Z} = \{ \phi_i \otimes \chi_i^* \}$. $Z$ may be the complete set of zeros of $\Omega$, or only a subset. The orthogonal complement $Z^\perp$ is a $d_1$ dimensional subspace of $\mathcal{H}$, and $\tilde{Z}^\perp$ is a $d_2$ dimensional subspace, with
\(d_1 \geq N - k\) and \(d_2 \geq N - k\). Let \(P\) and \(\tilde{P}\) be the orthogonal projections onto \(Z^\perp\) and \(\tilde{Z}^\perp\), respectively.

Define orthogonal projections \(P\) and \(\tilde{P}\) on the real Hilbert space \(H\) such that \(PX = PXP\) and \(\tilde{P}X = (\tilde{P}XP\tilde{P})\tilde{P}\) for \(X \in H\). Define the overlap of these two projections as the orthogonal projection \(O\) onto the subspace \((PH) \cap (\tilde{P}H)\). Since \(OX = X\) if and only if \(PX = X\) and \(\tilde{PX} = X\), we may compute \(O\) numerically by picking out the eigenvectors of \(P + \tilde{P}\) with eigenvalue 2. It follows that

\[
O = PO = OP = \tilde{P}O = O\tilde{P},
\]
and that \(P' = P - O\) and \(\tilde{P}' = \tilde{P} - O\) are orthogonal projections.

If \(\Omega = \rho + \sigma^P\) with \(\rho, \sigma \in D\), then we must have \(Z \subset \ker \rho\) and \(\tilde{Z} \subset \ker \sigma\), hence \(P\rho = \rho\) and \(P\sigma^P = (\tilde{P}\sigma\tilde{P})\tilde{P} = \sigma^P\). Defining \(\rho_1 = P'\rho\), \(\rho_2 = O\rho\), \(\sigma^P_1 = P'\sigma^P\), \(\sigma^P_2 = O\sigma^P\) we have that

\[
\Omega = \rho_1 + \rho_2 + \sigma^P_2 + \sigma^P_1
\]
with \(\rho_1 \in P'H\), \(\sigma^P_1 \in \tilde{P}'H\), and \(\rho_2 + \sigma^P_2 \in OH\). It follows that

\[
\rho_1 + \sigma^P_1 = \Omega - O\Omega, \quad \rho_2 + \sigma^P_2 = O\Omega.
\]

The decomposition of \(\Omega - O\Omega\) into \(\rho_1\) and \(\sigma^P_1\) is unique and easily computed.

If the overlap \(O\) is zero, then \(\rho_2 = 0\), \(\sigma_2 = 0\), and this is the end of the story, except that we should check that both \(\rho_1\) and \(\sigma_1\) are positive semidefinite. Otherwise it remains to decompose \(O\Omega\) into \(\rho_2\) and \(\sigma^P_2\) in such a way that \(\rho = \rho_1 + \rho_2\) and \(\sigma = \sigma_1 + \sigma_2\) are both positive semidefinite. This is the difficult part of the problem, and the solution, if it exists, need not be unique.

We have not pursued the problem further. To do so one should use the equations (47) and (49), which put strong and presumably useful restrictions on \(\rho\) and \(\sigma\). For any product vector \(\phi \otimes \chi\) and any \(\phi_i \otimes \chi_i \in Z\) it is required that

\[
(\phi \otimes \chi)\rho(\phi_i \otimes \chi_i) = (\phi \otimes \chi_i)\Omega(\phi_i \otimes \chi),
\]

\[
(\phi \otimes \chi^*_i)\sigma(\phi_i \otimes \chi^*) = (\phi \otimes \chi^*_i)\Omega^P(\phi_i \otimes \chi^*).
\]

### 5.4 Decomposable witnesses with prescribed zeros

One use of decomposable witnesses is that they provide examples of witnesses with prescribed zeros. We will describe now how this works, and we use the same notation as in the previous subsection.

Let \(\Omega = \rho + \sigma^P\) be a decomposable witness, as before. The necessary and sufficient conditions for \(\Omega\) to have \(Z\) as a predefined set of zeros is that \(\rho = UU^\dagger\) and \(\sigma = VV^\dagger\) with \(X, Y \in H\), \(U = PX\), \(V = \tilde{P}Y\). We choose \(\rho\) and \(\sigma\) to have the maximal ranks

\[
\text{rank } \rho = d_1, \quad \text{rank } \sigma = d_2,
\]

where \(d_1 \geq N - k\) and \(d_2 \geq N - k\) are the dimensions of \(Z^\perp\) and \(\tilde{Z}^\perp\) respectively. In the generic case, when \(k < N\) there will be no linear dependencies between the zeros, or between their partial conjugates, so that we will have \(d_1 = d_2 = N - k\).

The set of unnormalized decomposable witnesses of this form has dimension

\[
d_D = \text{rank } P' + \text{rank } \tilde{P}' + \text{rank } O = \text{rank } P + \text{rank } \tilde{P} - \text{rank } O = d_1^2 + d_2^2 - \text{rank } O.
\]
The corresponding set of normalized witnesses is a convex subset \( \mathcal{F}_D \subset \mathcal{F}_\Omega \) of dimension \( d_D - 1 \), consisting of witnesses of the form \( \Omega + t \Gamma \) with
\[
\Gamma = A + B \mathbf{P}, \quad \mathbf{P} A = A, \quad \bar{\mathbf{P}}(B \mathbf{P}) = B \mathbf{P}, \quad \text{Tr} \ A = \text{Tr} \ B = 0. \tag{64}
\]
These conditions ensure that \( \rho + tA \) and \( \sigma + tB \) will remain positive for small enough positive or negative finite values of the real parameter \( t \).

The witness \( \Omega \) is an interior point of a unique face of \( S_1^{\circ} \), which we call \( F_\Omega \), as defined in equation (42). The dimension of this face is \( d_\Omega - 1 \) when we define
\[
d_\Omega = \dim \text{Ker} \ U_\Omega. \tag{65}
\]

For a quadratic witness \( \Omega \) a lower limit is
\[
d_\Omega \geq N^2 - k M_2 \quad \text{with} \quad M_2 = 2(N_a + N_b) - 3. \tag{66}
\]
This inequality will usually be an equality, especially when \( k \) is small.

Since \( \mathcal{F}_D \subset \mathcal{F}_\Omega \) we must have \( d_D \leq d_\Omega \), implying a lower bound for the overlap \( \mathbf{O} \),
\[
\text{rank} \ \mathbf{O} \geq d_1^2 + d_2^2 - d_\Omega \geq 2(N - k)^2 - d_\Omega. \tag{67}
\]
In particular, when the inequality in equation (66) is an equality we have the nontrivial lower bound
\[
\text{rank} \ \mathbf{O} \geq N^2 - k(4N - 2k - M_2). \tag{68}
\]
The generic case when \( k \) is small is that \( d_D = d_\Omega \), which means that \( \text{rank} \ \mathbf{O} \) has the minimal value allowed by this inequality. See Table 2 where we have tabulated some values for \( d_D \) and \( d_\Omega \) found numerically.

When we prescribe \( k \) zeros of the decomposable witness \( \Omega \), there is a possibility that the actual number of zeros, \( k' \), is larger than \( k \). A simple counting exercise indicates how many zeros to expect. A product vector \( \phi \otimes \chi \) is a zero if and only if \( \rho(\phi \otimes \chi) = 0 \) and \( \sigma(\phi \otimes \chi^*) = 0 \). These are \( 2(N - k) \) complex equations for \( \phi \otimes \chi \). There are \( N_a + N_b - 2 \) complex degrees of freedom in a product vector, up to normalization of each factor. The critical value \( k = k_c \) is the number of zeros for which the number of equations equals the number of variables, \( i.e. \),
\[
k_c = N + 1 - \frac{N_a + N_b}{2}. \tag{69}
\]
We expect to find
\[
k' = k \quad \text{if} \quad k < k_c, \quad k' \geq k \quad \text{if} \quad k = k_c, \quad k' = \infty \quad \text{if} \quad k > k_c. \tag{70}
\]

Whether \( \Omega \) will be quadratic or quartic can be estimated as follows. The Hessian \( G_\Omega \) at a zero of \( \Omega \) is a real square matrix of dimension \( 2(N_a + N_b - 2) \). If \( \text{rank} \ \rho = d_1 \) and \( \text{rank} \ \sigma = d_2 \), then we may write \( \Omega = \rho + \sigma \mathbf{P} \) as a convex combination of \( d_1 + d_2 \) or fewer extremal decomposable witnesses. Each extremal decomposable witness contributes at most two nonzero eigenvalues to \( G_\Omega \). Thus, if we define \( d_H \) as the minimal dimension of the kernel of \( G_\Omega \) at any zero, we have a lower bound
\[
d_H \geq 2(N_a + N_b - d_1 - d_2 - 2). \tag{71}
\]
In Table 2 we list some numbers related to decomposable witnesses, for different dimensions $N_a \times N_b$. The numbers presented were obtained numerically as follows. We choose $k$ random product vectors. When $k < N$ there will exist decomposable witnesses with these as zeros, and $d_D$ is the computed dimension of the set of such witnesses. $k'$ is the actual number of zeros they have. The listed value of $d_\Omega$, the dimension of the kernel of $U_\Omega$ when $\Omega$ is a quadratic witness with these zeros, is the lower bound given in equation (66). The listed value of the dimension $d_H$ of the kernel of the Hessian is the lower bound from equation (71).

We see from the table that with only a few zeros, the set of decomposable witnesses in the face has the same dimension as the face itself. But $F_\Omega$ can not consist entirely of decomposable witnesses, because in that case our numerical searches for extremal witnesses, where we search for witnesses with increasing numbers of zeros, would only produce decomposable witnesses, exactly the opposite of what actually happens. Hence we conclude that $F_D$ is a closed subset of $F_\Omega$, of the same dimension as $F_\Omega$ but strictly smaller than $F_\Omega$.

On a face defined by a higher number of zeros the set of decomposable witnesses has a lower dimension. In some cases the decomposable witnesses will lie on the boundary of the face in question. This will either be because they have more than $k$ zeros, or because some of the $k$ zeros are quartic. In other cases the decomposable witnesses make up a low dimensional part of the interior of the quadratic face. This is the case e.g. for faces $F_4$ in $3 \times 3$ systems, where the set of decomposable witnesses is 44 dimensional, the face is 45 dimensional, and the decomposable witnesses have 4 quadratic zeros and hence are situated in the interior of the face.

6 Examples of extremal witnesses

In this section we apply Theorem 4.5 and Algorithm 1 to study examples of extremal witnesses. We study first examples known from the literature, in particular the Choi–Lam witness [21,22] and the Robertson witness [23]. In Subsections 6.3, 6.3.1, and 6.3.2 we construct numerical examples of generic witnesses, study these and report some observations. Finally, in Subsection 6.3.3 we present an example of a nongeneric extremal witness, numerically constructed, having more than the minimum number of zeros.

6.1 The Choi–Lam witness

Define, like in [27],

$$\Omega_K(a, b, c; \theta) = \begin{pmatrix}
 a & \ldots & -e^{i\theta} & \ldots & -e^{-i\theta} \\
 \cdot & c & \ldots & \cdot & \cdot \\
 \cdot & \cdot & b & \ldots & \cdot \\
 -e^{-i\theta} & \cdot & \cdot & a & -e^{i\theta} \\
 \cdot & \cdot & \cdot & c & \cdot \\
 \cdot & \cdot & \cdot & \cdot & b \\
 -e^{i\theta} & \cdot & \cdot & -e^{-i\theta} & \cdot \\
 \cdot & \cdot & \cdot & \cdot & a
\end{pmatrix}. \quad (72)$$

We write dots instead of zeros in the matrix to make it more readable. The special case $\Omega_C = \Omega_K(1, 0, 1; 0)$ is the Choi–Lam witness, one of the first examples of a nondecomposable
Table 2: Numbers related to decomposable witnesses, as explained in the text. $k$ is the prescribed number of zeros and $k'$ is the actual number, which may be larger. $k_c$ is the critical number of prescribed zeros for which we expect a finite number of zeros in total. If $k < k_c$ we expect only the prescribed zeros. If $k = k_c$ we expect some finite number of zeros. If $k > k_c$ we expect a continuum of zeros.

| $N_a \times N_b$ | $k$ | $k'$ | $d_D$ | $d_\Omega$ | $d_H$ |
|-------------------|-----|------|-------|------------|------|
| 2 $\times$ 4     | 1   | 1    | 55    | 55         | 0    |
| $k_c = 6$         | 2   | 2    | 46    | 46         | 0    |
|                   | 3   | 3    | 37    | 37         | 0    |
|                   | 4   | 4    | 28    | 28         | 0    |
|                   | 5   | 5    | 18    | 19         | 2    |
|                   | 6   | 8    | 10    | 4          |      |
|                   | 7   | $\infty$ | 2  | 2         | 6    |
| 3 $\times$ 3     | 1   | 1    | 72    | 72         | 0    |
| $k_c = 7$         | 2   | 2    | 63    | 63         | 0    |
|                   | 3   | 3    | 54    | 54         | 0    |
|                   | 4   | 4    | 44    | 45         | 0    |
|                   | 5   | 5    | 32    | 36         | 0    |
|                   | 6   | 6    | 18    | 27         | 2    |
|                   | 7   | 10,14| 8    | 18         | 4    |
|                   | 8   | $\infty$ | 2  | 9         | 6    |
| 3 $\times$ 4     | 1   | 1    | 133   | 133        | 0    |
| $k_c = 9.5$       | 2   | 2    | 122   | 122        | 0    |
|                   | 3   | 3    | 111   | 111        | 0    |
|                   | 4   | 4    | 100   | 100        | 0    |
|                   | 5   | 5    | 88    | 89         | 0    |
|                   | 6   | 6    | 72    | 78         | 0    |
|                   | 7   | 7    | 50    | 67         | 2    |
|                   | 8   | 8    | 32    | 56         | 4    |
|                   | 9   | 9    | 18    | 45         | 6    |
|                   | 10  | $\infty$ | 8   | 34         | 8    |
|                   | 11  | $\infty$ | 2   | 23         | 10   |
|                   | 12  | $-$   | 0    | 12         | $-$  |

The set of zeros of $\Omega_C$ consists of three isolated quartic zeros

$$e_{13} = e_1 \otimes e_3, \quad e_{21} = e_2 \otimes e_1, \quad e_{32} = e_3 \otimes e_2,$$

where $e_1, e_2, e_3$ are the natural basis vectors in $\mathbb{C}^3$, and a continuum of zeros $\phi \otimes \chi$ where $\alpha, \beta \in \mathbb{R}$ and

$$\phi = e_1 + e^{i\alpha} e_2 + e^{i\beta} e_3, \quad \chi = \phi^*.$$

The product vectors defined in equation (74) span a seven dimensional subspace consisting of all vectors $\psi \in \mathbb{C}^9$ with components $\psi_1 = \psi_5 = \psi_9 = 0$. The three product vectors defined in equation (73) have $\psi_1 = \psi_5 = \psi_9 = 0$ and lie in the same subspace.
The Hessian has a doubly degenerate kernel at each of these zeros. Hence, a single zero of \( \Omega = \Omega_C \) contributes 29 equations in \( U_\Omega \): 9 from \( T_0 \) and \( T_1 \), \( 2 \times 8 \) from \( T_2 \), and 4 from \( T_3 \). However, by a singular value decomposition of \( T = T_0 \oplus T_1 \oplus T_2 \oplus T_3 \) at one zero at a time we find numerically that the number of independent equations is 24 for each of the isolated zeros and 28 for any randomly chosen nonisolated zero. We again see that redundant equations appear when the kernel of the Hessian is more than one dimensional. We also observe that the redundancies depend on the nature of the zero.

Choosing increasingly many nonisolated zeros, only 67 linearly independent equations are obtained, out of the 80 needed for proving extremality. These 67 equations are obtained with the quadratic and quartic constraints from three zeros, or with only the quadratic constraints from nine zeros. With all three isolated zeros and any single zero from the continuum, \( \text{Ker } U_\Omega \) is one dimensional and uniquely defines the Choi–Lam witness. This verifies numerically that it is extremal. We need the quartic constraints from the three isolated zeros in order to prove extremality, because the quadratic constraints from all the zeros provide only 76 independent equations, leaving a four dimensional face of witnesses having the same set of zeros as the Choi–Lam witness \( \Omega_C \). This proves that \( \Omega_C \) is not exposed, but is an extremal point of a four dimensional exposed face of \( S^1_\Omega \).

Equation (72) with \( \theta = 0 \) and the restrictions \( 0 \leq a \leq 1, \ a + b + c = 2, \ bc = (1 - a)^2 \), defines more generally a one parameter family of extremal witnesses considered by Ha and Kye [51, 52]. They prove that \( \Omega_K(a,b,c;0) \) is both extremal and exposed for \( 0 < a < 1 \). The original Choi–Lam witness \( \Omega_C \) is extremal but not exposed, it is the limiting case \( a = c = 1, \ b = 0 \). We will return in Section 8 to a more detailed discussion of the facial structure of the set of separable states and the set of witnesses.

We have verified by our numerical methods, for several values of \( a \) with \( 0 < a < 1 \), that \( \Omega_K(a,b,c;0) \) is indeed extremal. As explained in [52] there are four classes of zeros. The zeros in one of these classes have Hessians with two dimensional kernels, while the Hessians of the zeros in the other three classes have one dimensional kernels. It turns out that a set of four zeros, one from each class, uniquely defines \( \Omega_K(a,b,c;0) \) as the only solution to the constraints imposed by the zeros when utilizing both quadratic and quartic constraints. This shows numerically that the witness is extremal.

### 6.2 The Robertson witness

Another example we have studied is the extremal positive map in dimension \( 4 \times 4 \) introduced by Robertson [23],

\[
X \rightarrow \begin{pmatrix}
X_{33} + X_{44} & 0 & X_{13} + X_{42} & X_{14} - X_{32} \\
0 & X_{33} + X_{44} & X_{23} - X_{41} & X_{24} + X_{31} \\
X_{31} + X_{24} & X_{32} - X_{14} & X_{11} + X_{22} & 0 \\
X_{41} - X_{23} & X_{42} + X_{13} & 0 & X_{11} + X_{22}
\end{pmatrix}.
\]  

(75)
By equation (9), it corresponds to the witness

\[
\Omega_R = \begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & -1 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\end{pmatrix}.
\]  

(76)

The corresponding biquadratic form is

\[
f_R(\phi, \chi) = (|\phi_1|^2 + |\phi_2|^2)(|\chi_3|^2 + |\chi_4|^2) + (|\phi_3|^2 + |\phi_4|^2)(|\chi_1|^2 + |\chi_2|^2)
+ 2 \text{Re} \left[ (\phi_1^* \phi_3 + \phi_2^* \phi_2)(\chi_3^* \chi_1 + \chi_2^* \chi_4) + (\phi_2^* \phi_3 - \phi_4^* \phi_1)(\chi_3^* \chi_2 - \chi_1^* \chi_4) \right].
\]  

(77)

Every product vector \(\phi \otimes \chi\) with \(\phi_1 = \phi_2 = \chi_1 = \chi_2 = 0\) or \(\phi_3 = \phi_4 = \chi_3 = \chi_4 = 0\) is a zero. More generally, \(\phi \otimes \chi\) is a zero if

\[
(|\phi_1|^2 + |\phi_2|^2)(|\chi_3|^2 + |\chi_4|^2) = (|\phi_3|^2 + |\phi_4|^2)(|\chi_1|^2 + |\chi_2|^2)
\]  

(78)

and

\[
\phi_1^* \phi_3 + \phi_4^* \phi_2 = -\chi_1^* \chi_3 - \chi_4^* \chi_2 ,
\phi_2^* \phi_3 - \phi_4^* \phi_1 = -\chi_2^* \chi_3 + \chi_4^* \chi_1 .
\]  

(79)

For any given \(\phi\) we obtain a continuum of zeros in the following way. Define

\[
a = \phi_1^* \phi_3 + \phi_4^* \phi_2 , \quad b = \phi_2^* \phi_3 - \phi_4^* \phi_1 .
\]  

(80)

Then choose \(\chi_1, \chi_2\) at random and define

\[
\chi_3 = \frac{-a \chi_1 - b \chi_2}{|\chi_1|^2 + |\chi_2|^2} , \quad \chi_4 = \frac{b^* \chi_1 - a^* \chi_2}{|\chi_1|^2 + |\chi_2|^2} .
\]  

(81)

This solves equation (79). In order to solve also equation (78), rescale \(\chi_i \rightarrow c \chi_i\) for \(i = 1, 2\) and \(\chi_i \rightarrow \chi_i/c\) for \(i = 3, 4\) with a suitably chosen constant \(c > 0\).

We have verified numerically that \(\Omega_R\) is extremal. Four zeros determine the witness uniquely through the quadratic and quartic constraints, e.g. the zeros

\[
e_{ij} = e_i \otimes e_j , \quad ij = 11, 12, 33, 34 .
\]  

(82)
It appears that all zeros have Hessians with eight dimensional kernels. The witness has a continuum of zeros, and 20 randomly chosen of these turn out to also uniquely determine the witness through only quadratic constraints. The fact that the quadratic constraints are sufficient to determine the witness uniquely proves that it is exposed. See Section 8 for a discussion of exposed faces.

As a related example we have looked at a witness $\Omega_Z$ belonging to a new class of witnesses in dimension $N \times (2K)$ introduced by Zwolak and Chruściński [28, 53, 54]. We take $N = 2$, $K = 1$, and $|z_{12}| = 1$ in their notation. Structurally similar to $\Omega_R$, $\Omega_Z$ also has the zeros defined in equation (82), and again the quadratic and quartic constraints from these four zeros determine $\Omega_Z$ uniquely. This verifies numerically that $\Omega_Z$ is extremal, and exemplifies the fact that the same set of zeros with different Hessian zeros can uniquely specify two different witnesses. This witness, like $\Omega_R$, has a continuous set of zeros and can be determined uniquely through only the quadratic constraints from a randomly chosen set of 20 of these zeros. Hence it is exposed.

### 6.3 Numerical examples, generic and nongeneric

We have successfully implemented Algorithm 1 and used it to locate numerical examples of extremal witnesses in $2 \times 4$, $3 \times 3$ and $3 \times 4$ dimensions. In the process of searching for an extremal witness we produce witnesses situated on a hierarchy of successively lower dimensional faces of $S_0^1$.

We define a class of extremal witnesses to be generic if such witnesses can be found with nonzero probability by means of Algorithm 1 when the search direction $\Gamma$ is chosen at random in every iteration. An overwhelming majority of the extremal witnesses found in numerical random searches are quadratic, but a small number of quartic witnesses are also found. There may be numerical problems in locating a zero which is quartic or close to quartic. In such cases our implementation of the algorithm stops prematurely. We discuss the quartic witnesses in Subsection 6.3.2.

Line 5 of Algorithm 1 regards locating the boundary of a face. Appendix B.2 describes how this can be formulated as a problem of locating a simple root of a special function, and also mentions other possible approaches.

#### 6.3.1 Quadratic extremal witnesses

We make the following comments concerning the quadratic extremal witnesses found.

- We have experienced premature stops due to numerical problems with zeros that are close to quartic. See further comments in Subsection 6.3.2.

- When no existing zero becomes close to quartic, a single new quadratic zero appears in every iteration of Algorithm 1 when the boundary of the current face is reached. For a small number of zeros, there is no redundancy between constraints from the existing zeros and constraints from the new zero. A redundancy appears typically with the seventh zero in $2 \times 4$, with the ninth zero in $3 \times 3$, and never in $3 \times 4$. This gives a hierarchy of faces of $S_0^1$ of dimension $N^2 - 1 - kM_2$, where $k$ is the number of zeros of a witness in the interior of the face, and $M_2 = 2(N_a + N_b) - 3$.

- The extremal witnesses have the expected number of zeros as listed in Table 1. The zeros and the partially conjugated zeros span $\mathcal{H}$, as required by Theorem 4.6.
# negative eigenvalues for witnesses \((\Omega, \Omega^P)\)

### Table 3: Classification of generic quadratic extremal witnesses, obtained by Algorithm 1, in dimensions \(3 \times 3\) and \(3 \times 4\). A witness and its partial transpose has respectively \(p\) and \(q\) negative eigenvalues. The table lists the number of witnesses found.

| \((p, q)\) | \(3 \times 3\) | \(3 \times 4\) |
|-----------|----------------|----------------|
| \((1, 2)/(2, 1)\) | 0/1 | 0/0 |
| \((2, 2)\) | 98 | 1 |
| \((2, 3)/(3, 2)\) | 27/37 | 3/4 |
| \((3, 3)\) | 8 | 47 |
| \((3, 4)/(4, 3)\) | 0/0 | 4/6 |

- A quadratic extremal witness has at least one negative eigenvalue, and the same is true for its partial transpose. We do not find extremal witnesses with more than 3 negative eigenvalues in \(3 \times 3\) or more than 4 negative eigenvalues in \(3 \times 4\). See Table 3 and Figure 2.
- Every witness and its partial transpose have full rank.

### 6.3.2 Quartic extremal witnesses

In each iteration of Algorithm 1 the critical parameter value \(t_c\) is reached when either a new quadratic zero appears, or a new zero eigenvalue of the Hessian matrix appears at one of the
existing zeros. If the second alternative occurs at least once during a search, then the extremal witness found will be quartic, otherwise it will be quadratic. Our experience is that a random search most often produces a quadratic extremal witness and only rarely a quartic extremal witness.

In order to make this observation more quantitative we have made random searches for quartic witnesses in dimension $3 \times 3$ as follows. We take 58 hierarchies of faces of quadratic witnesses generated by Algorithm 1, and generate 100 random perturbations $\Gamma$ away from the quadratic witness found on each face. Since there are 8 faces in each of the 58 hierarchies, this is a total of 46400 tests. For each test we compute $t_c'$ as the smallest $t$ resulting in a zero eigenvalue of the Hessian at a zero. $t_c'$ is thus an upper bound for $t_c$. At $t = t_c'$ we test whether $\Omega + t\Gamma$ is still a witness, in which case it has got a quartic zero, or if it is no longer a witness, which will mean that there has appeared a new quadratic zero for some $t < t_c'$. 3 runs failed, probably due to some bug in the algorithm. With a tolerance of $\pm 10^{-14}$ on function values we found that only 91 out of 46397 successful tests resulted in quartic witnesses. Thus, in this quantitative test the probability for finding a quartic witness was 0.2%. We conclude that the fraction of quartic extremal witnesses among the generic extremal witnesses is small but nonzero.

We constructed an explicit example of a quartic extremal witness in $3 \times 3$ with 8 zeros in the following way. Starting at a quadratic witness on a face $\mathcal{F}_4$ generated by Algorithm 1 we found a quartic witness on the boundary of $\mathcal{F}_4$ by choosing one quadratic zero to become quartic and perturbing the quadratic witness accordingly. (This may not succeed, in which case we choose a different zero.) Continuing Algorithm 1 from this quartic witness resulted in an extremal witness with 8 zeros, of which one is a quartic zero with a one dimensional kernel of the Hessian. Running Algorithm 1 succeeded since we knew priori which zero was quartic, so problems with the numerical precision could be overcome. We observe that as $M_2 = 9$ constraints from each of the 6 first quadratic zeros are added to $U_{\Omega 1}$, and further as $M_2 + M_4(1) = 18$ constraints from the quartic zero are added to form $U_\Omega$, all of these are linearly independent. Hence $U_\Omega$ has rank 72 as expected, and a single new quadratic zero is located in the final step, adding 8 new linearly independent constraints so as to make $\dim \ker U_\Omega = 1$.

### 6.3.3 Nongeneric quadratic extremal witnesses

In order to demonstrate that a quadratic extremal witness may have more than the minimum number of zeros, we have constructed quadratic extremal witnesses in $3 \times 3$ dimensions with 10 rather than the expected number of 9 zeros.

One method for finding such witnesses is illustrated in Figure 4, where the kink in the curve to the right represents a witness with 10 zeros. All witnesses on the face have 8 zeros in common, whereas the curved lines on both sides of the kink consist of quadratic extremal witnesses with 9 zeros. We will return to this example in the next section.

An entirely different method is described here. The basic idea is to use Theorem 4.6 and try to construct 9 product vectors $\psi_i = \phi_i \otimes \chi_i$ that are linearly dependent, and for good measure such that also the partially conjugated product vectors $\tilde{\psi}_i = \phi_i \otimes \chi_i^*$ are linearly dependent. Then a quadratic witness with these 9 zeros, and no more, can not be extremal, but it might lead to a quadratic extremal witness with 10 zeros.

A first attempt is to choose the 9 product vectors directly, by minimizing the sum of the smallest singular value of the $9 \times 9$ matrix $\Psi = [\psi_1, \psi_2, \ldots, \psi_9]$ and the smallest singular value
of the corresponding $9 \times 9$ matrix $\tilde{\psi}$. Since singular values are nonnegative by definition, minimization will make both these singular values zero. The minimization problem is solved e.g. by the Nelder–Mead algorithm, or by a random search.

Let $Z$ be a set of 9 product vectors generated in this way, then any witness $\Omega$ with these as zeros has to satisfy the constraints $U_{01} \Omega = 0$. The generic result we find is that $\dim \ker U_{01} = 2$. Hence $\Omega$ has to be a decomposable witness,$$
abla^* \Omega = p \eta \eta^\dagger + (1-p) (\eta \eta^\dagger)^P, \tag{83}
$$
with $\eta, \tilde{\eta} \in \mathcal{H}$, $\eta^\dagger \psi_i = \tilde{\eta}^\dagger \tilde{\psi}_i = 0$ for $i = 1, \ldots, 9$, and $0 \leq p \leq 1$. This decomposable $\Omega$ is not what we are looking for, in fact it has a continuum of quartic zeros. The extremal decomposable witnesses $\eta \eta^\dagger$ and $(\eta \eta^\dagger)^P$ each contribute two nonzero eigenvalues to the $8 \times 8$ Hessian matrix $G_{\Omega}$ at every zero, hence $\dim \ker G_{\Omega} = 4$ at every zero, unless $p = 0$ or $p = 1$ in which case $\dim \ker G_{\Omega} = 6$.

A second attempt is to choose 8 product vectors $\psi_i$ that are linearly dependent and have linearly dependent partial conjugates $\tilde{\psi}_i$. This almost works, but not quite. We may construct a decomposable witness $\Omega$ with these zeros from two pure states orthogonal to all $\psi_i$ and two partially transposed pure states orthogonal to all $\tilde{\psi}_i$. As a convex combination of four extremal decomposable witnesses, each contributing two nonzero eigenvalues to each $8 \times 8$ Hessian matrix, $\Omega$ will be quadratic. $\Omega$ is determined by 8 real parameters, including a normalization constant, since $\Omega = \rho + \sigma^P$ where $\rho$ and $\sigma$ are positive matrices of rank two, with $\rho \psi_i = \sigma \tilde{\psi}_i = 0$. The maximum number of independent constraints from 8 quadratic zeros is 72, giving $\dim \ker U_{01} = 9$, one more than the dimension of the set of decomposable witnesses having these zeros. However, we find that $\Omega$ generically has more than the 8 prescribed zeros, increasing the number of independent constraints to 73. Hence, again the constraints leave only the decomposable witnesses, none of which are quadratic and extremal.

The third and successful attempt is to choose 7 product vectors with similar linear dependencies. Denote by $U_{01}^{(7)}$ the corresponding linear system of constraints. The kernel of $U_{01}^{(7)}$ is found, in two different cases, to have dimension 21 or 22. A decomposable witness with the given product vectors as zeros has the form $\Omega_7 = \rho + \sigma^P$ where $\rho$ and $\sigma$ are positive matrices of rank three. Hence, the set of such decomposable witnesses is 18 dimensional, so that there are 3 or 4 dimensions in $\ker U_{01}^{(7)}$ orthogonal to the face of decomposable witnesses. Defining $\Gamma_7$ to lie in these 3 or 4 dimensions one can walk towards the boundary of the face $\mathcal{F}_7 = (\ker U_{01}^{(7)}) \cap \mathcal{S}_1^0$, finding $\Omega_8 = \Omega_7 + t_\gamma \Gamma_7$ with 8 zeros. $\Omega_8$ is now guaranteed to be nondecomposable. Let $U_{01}^{(8)}$ be the system defined by these 8 zeros, defining the face $\mathcal{F}_8 = (\ker U_{01}^{(8)}) \cap \mathcal{S}_1^0$. We find that $\ker U_{01}^{(8)}$ has dimension 9 less than $\ker U_{01}^{(7)}$. Defining $\gamma_8 \in \ker U_{01}^{(8)}$, we locate an $\Omega_9 \in \mathcal{F}_9$, on the boundary of $\mathcal{F}_8$, with 9 zeros. The kernel of $U_{01}^{(9)}$ has dimension 9 less than $\ker U_{01}^{(8)}$, i.e. 3 or 4, hence there is still freedom to move along $\mathcal{F}_9$. Doing so produces a quadratic extremal witness in $3 \times 3$ with 10 zeros rather than 9.

### 7 D-shaped faces of the set of witnesses in low dimensions

In this section we reveal a special geometry of next-to-extremal faces of $\mathcal{S}_1^0$ in $2 \times 4$ and $3 \times 3$ systems, related to the presence of decomposable witnesses.

Let $\mathcal{F}_k$ denote a face of $\mathcal{S}_1^0$ with interior points that are quadratic witnesses with $k$ zeros. This is typically what we find in the $k$-th iteration of Algorithm 1. A face $\mathcal{F}_7$ in dimension
Figure 3: A two dimensional face \( \mathcal{F}_7 \subset S_0^7 \) obtained by applying Algorithm 1 in dimension \( 2 \times 4 \). Distances are defined by the Hilbert–Schmidt metric. The straight line segment (dashed, in red) consists of decomposable witnesses, its upper end point is a pure state, marked by a diamond, and its lower end point is the partial transpose of a pure state, marked by a circle. Starting from a quadratic witness with seven zeros, marked by the black dot, the curved boundary of the face (in blue) was located by perturbing in all directions. Every point on this curve represents an extremal witness with eight quadratic zeros, except at the kink in the middle of the curved boundary where the witness has nine quadratic zeros. These extremal witnesses are very nearly quartic. We show this by drawing another curved line (dashed, in blue) where the first Hessian zero appears, that is, where one zero becomes quartic. This dashed curve is only visible in the enlarged part of the figure.

\( 2 \times 4 \), or \( \mathcal{F}_8 \) in dimension \( 3 \times 3 \), is the last face found before an extremal quadratic witness is reached. These particular faces have a special geometry, because the number of zeros is one less than the dimension of the Hilbert space, and as a result part of the boundary is a line segment of decomposable witnesses.

A decomposable witness on such a face has the form

\[
\Omega = (1 - p) \psi \psi^\dagger + p (\eta \eta^\dagger)^p, \quad 0 \leq p \leq 1,
\]

where \( \psi \) is orthogonal to the \( N - 1 \) product vectors \( \phi_i \otimes \chi_i \) that are the zeros of all the witnesses in the interior of the face, and \( \eta \) is orthogonal to the partially conjugated product vectors \( \phi_i \otimes \chi_i^\dagger \). We take \( \psi \) and \( \eta \) to be normalized vectors, \( \psi^\dagger \psi = \eta^\dagger \eta = 1 \).

When we apply Algorithm 1 in \( 2 \times 4 \) dimensions and find a quadratic extremal witness, the generic case is that the face \( \mathcal{F}_7 \) is two dimensional. An example is shown in Figure 3. The line segment of decomposable witnesses must be part of the boundary of the face \( \mathcal{F}_7 \), because the interior of the face consists of quadratic witnesses with a fixed set of 7 quadratic zeros, whereas the decomposable witnesses have additional zeros and Hessian zeros, in fact infinitely many quartic zeros. The rest of the boundary of the face is curved, and consists of quadratic extremal witnesses with 8 zeros. There is one exception, however, seen in the figure as a kink in the curved part of the boundary, and this is a quadratic extremal witness with 9 zeros.
The interesting explanation is as follows. As we go along the curve consisting of quadratic witnesses with 8 zeros, 7 zeros are fixed, they are the zeros defining the face. But the 8th zero has to change along the curve, because any two points on this part of the boundary can be joined by a line segment passing through the interior of the face, hence these two boundary points can have only the 7 zeros in common. Starting from the two extremal decomposable witnesses $\psi\psi^\dagger$ and $\eta\eta^\dagger$ we get two curved sections of the boundary where the 8th zero changes continuously. These two sections meet in one point which is then a witness with two quadratic zeros in addition to the 7 zeros defining the face.

Accordingly, this next-to-extremal face $\mathcal{F}_7$ is two dimensional and has the shape of a “D”, where the straight edge is the line segment of decomposable witnesses and the round part consists of quadratic extremal witnesses. Figure 3 is a numerically produced example of such a face. Along similar lines we expect that next-to-extremal faces in any $2 \times N_b$ systems will be either D-shaped, or line segments if by accident we hit the straight edge of the D.

In the case of $\mathcal{F}_8$ in $3 \times 3$ we can also construct the line segment of decomposable witnesses on the boundary of $\mathcal{F}_8$. The remaining boundary will again consist of quadratic extremal witnesses, this time with 9 or 10 zeros. This part of the boundary is a curved 7 dimensional surface, since the face itself is 8 dimensional. Any two dimensional section of $\mathcal{F}_8$ passing through the line segment of decomposable witnesses is shaped as a D. See Figure 4 for a numerically computed example.

Note that we can not guarantee that any choice of 8 random product vectors gives rise to such a D. Many choices may give rise to only the line segment of decomposable witnesses, since there are inequality constraints that are not automatically satisfied, even if we are able to satisfy the equality constraints that we have discussed here.

In other dimensions line segments of decomposable witnesses constructed from $N - 1$ zeros also define D-shaped faces, but the round part of the “D” will in those cases consist not of extremal witnesses but of lower dimensional faces.

8  Faces of the set of separable states

Our understanding of witnesses as exposed in Section 4 translates into an understanding of faces of $S_1$, the set of separable states. A face of a compact convex set is defined by the extremal points it contains, and in the case of $S_1$ the extremal points are the pure product states. Alfsen and Shultz [16] describe faces of $S_1$ in two categories, either simplexes defined by at most $\max(N_a, N_b)$ pure product states, or direct convex sums of faces isomorphic to matrix algebras. According to our understanding these two categories correspond to quadratic and certain quartic witnesses respectively. It has been known for some time that the set of entanglement witnesses has unexposed faces. These questions have been studied by Chruściński and collaborators [28, 55]. In our understanding the unexposed faces of $S_1^o$ are those containing quartic witnesses as interior points. The facial structure of various sets related to quantum entanglement has been studied especially by Kye and collaborators [56].

In this section we describe faces of $S_1$ defined by different types of witnesses. We state some basic results which may be well known and which are actually quite generally valid for any pair of dual convex cones. The distinction between exposed and unexposed faces is central, and it would be interesting to know whether all the faces of the set of separable states are exposed. We believe that this is true, although we have no proof. Some support for our conjecture may be drawn from the known facts that both the set of density matrices and the
Figure 4: A special two dimensional section of an eight dimensional face $F_8 \subset S_1^0$ obtained from output of Algorithm 1 in dimension $3 \times 3$. This section passes through a straight line segment of decomposable witnesses (dashed, in red) which is part of the boundary of the face. The upper end point of the line segment is a pure state, marked by a diamond, and the lower end point is the partial transpose of a pure state, marked by a circle. Starting from a quadratic witness with eight zeros, marked by the black dot, the curved boundary of the face (in blue) was located by perturbing in all directions in the plane. Every point on this curve represents an extremal witness with nine quadratic zeros, except at the kink where the witness has ten zeros. The curved dashed line (in blue) is where one zero becomes quartic.

set of PPT states have only exposed faces.

To finish this section we point out how the facial structure of the set of separable states is related to a question which is of practical importance when we want to test whether a given state is separable. The question is how many pure product states we need, if the state is separable, in order to write it as a convex combination of pure product states.
8.1 Duality of faces

Given any subset $\mathcal{X} \subset S_1$ we define its dual in $S_1^\circ$ as

$$\mathcal{X}^\circ = \{ \Omega \in S_1^\circ \mid \text{Tr} \Omega \rho = 0 \ \forall \rho \in \mathcal{X} \}.$$  \hfill (84)

Similarly, given any subset $\mathcal{Y} \subset S_1^\circ$ we define its dual in $S_1$ as

$$\mathcal{Y}^\circ = \{ \rho \in S_1 \mid \text{Tr} \Omega \rho = 0 \ \forall \Omega \in \mathcal{Y} \}.$$  \hfill (85)

We will assume here that $\mathcal{X}^\circ$ and $\mathcal{Y}^\circ$ are nonempty, a minimum requirement is that $\mathcal{X} \subset \partial S_1$ and $\mathcal{Y} \subset \partial S_1^\circ$. Then also $\mathcal{X}^\circ \subset \partial S_1^\circ$ and $\mathcal{Y}^\circ \subset \partial S_1$.

There always exists one single $\rho_0 \in \partial S_1$ such that

$$\mathcal{X}^\circ = \{ \rho_0 \}^\circ = \{ \Omega \in S_1^\circ \mid \text{Tr} \Omega \rho_0 = 0 \}.$$  \hfill (86)

In fact, every $\rho \in \mathcal{X}$ gives one linear constraint $\text{Tr} \Omega \rho = 0$ as part of the definition of $\mathcal{X}^\circ$. In finite dimension at most a finite number of linear constraints can be independent, hence

$$\mathcal{X}^\circ = \{ \Omega \in S_1^\circ \mid \text{Tr} \Omega \rho_i = 0 \text{ for } i = 1, 2, \ldots, k \}.$$  \hfill (87)

for some states $\rho_1, \rho_2, \ldots, \rho_k \in \mathcal{X}$. Define for example

$$\rho_0 = \frac{1}{k} \sum_{i=1}^k \rho_i.$$  \hfill (88)

It may happen that $\rho_0 \notin \mathcal{X}$ if $\mathcal{X}$ is not convex. Because $\text{Tr} \Omega \rho_i \geq 0$ for $i = 1, 2, \ldots, k$ the equation $\text{Tr} \Omega \rho_0 = 0$ implies that $\text{Tr} \Omega \rho_i = 0$ for $i = 1, 2, \ldots, k$ and hence $\Omega \in \mathcal{X}^\circ$.

Taking three times the dual we get that $\mathcal{X}^\circ = \mathcal{F}^\circ$ where $\mathcal{F} = \mathcal{X}^{\circ\circ}$ is the double dual of $\mathcal{X}$. Clearly $\mathcal{F}$ contains $\mathcal{X}$, and by our next theorem $\mathcal{F}$ is an exposed face of $S_1$.

Reasoning in the same way we conclude that it is always possible to find one single witness $\Omega_0$ such that

$$\mathcal{Y}^\circ = \{ \Omega_0 \}^\circ = \{ \rho \in S_1 \mid \text{Tr} \Omega_0 \rho = 0 \},$$  \hfill (89)

and an exposed face $\mathcal{G}$ of $S_1^\circ$ containing $\mathcal{Y}$, in fact $\mathcal{G} = \mathcal{G}^{\circ\circ}$, such that $\mathcal{Y}^\circ = \mathcal{G}^\circ$.

**Theorem 8.1.** $\mathcal{X}^\circ$ is an exposed face of $S_1^\circ$, and $\mathcal{Y}^\circ$ is an exposed face of $S_1$.

*Proof.* Assume that $\Omega \in \mathcal{X}^\circ$ is a proper convex combination of $\Omega_1, \Omega_2 \in S_1^\circ$,

$$\Omega = (1 - p) \Omega_1 + p \Omega_2 \quad \text{with} \quad 0 < p < 1.$$  \hfill (90)

We have to prove that $\Omega_1, \Omega_2 \in \mathcal{X}^\circ$. The assumption that $\Omega_1, \Omega_2 \in S_1^\circ$ means that $\text{Tr} \Omega_1 \rho \geq 0$ and $\text{Tr} \Omega_2 \rho \geq 0$ for every $\rho \in S_1$. For every $\rho \in \mathcal{X}$ we have in addition that

$$0 = \text{Tr} \Omega \rho = (1 - p) \text{Tr} \Omega_1 \rho + p \text{Tr} \Omega_2 \rho,$$  \hfill (91)

and from this we conclude that $\text{Tr} \Omega_1 \rho = \text{Tr} \Omega_2 \rho = 0$. This proves that $\Omega_1, \Omega_2 \in \mathcal{X}^\circ$, so that $\mathcal{X}^\circ$ is a face.

It is exposed because it is dual to one single $\rho_0 \in S_1$. In fact, the equation $\text{Tr} \Lambda \rho_0 = 0$ for $\Lambda$ defines a hyperplane of dimension $N^2 - 2$ in the $N^2 - 1$ dimensional affine space of Hermitian $N \times N$ matrices of unit trace.

The proof that $\mathcal{Y}^\circ$ is an exposed face is entirely similar. \qed
This theorem has the following converse.

**Theorem 8.2.** An exposed face of $S^1_1$ is the dual of a separable state, and an exposed face of $S_1$ is the dual of a witness.

*Proof.* We prove the second half of the theorem, the first half is proved in a similar way.

An exposed face $F$ of $S_1$ is the intersection of $S_1$ with a hyperplane given by an equation for $\rho \in H$ of the form $\text{Tr} \Lambda \rho = 0$ where $\Lambda \in H$ is fixed. The maximally mixed state $\rho_0 = 1/N$ is an interior point of $S_1$, hence $\text{Tr} \Lambda = N \text{Tr} \Lambda \rho_0 \neq 0$ and we may impose the normalization condition $\text{Tr} \Lambda = 1$. We have to prove that $\Lambda \in S^1_1$, which means that $\text{Tr} \Lambda \rho \geq 0$ for all $\rho \in S_1$.

Assume that there exists some $\rho_1 \in S_1$ with $\text{Tr} \Lambda \rho_1 < 0$. Choose any $\rho_2 \in S_1$ with $\text{Tr} \Lambda \rho_2 > 0$, for example $\rho_2 = \rho_0$. Then $\rho_1, \rho_2 \notin F$, since $F$ is defined as the set of all $\rho \in S_1$ having $\text{Tr} \Lambda \rho = 0$. But there exists a proper convex combination $\rho = (1 - p)\rho_1 + p\rho_2$ with $0 < p < 1$ such that $\text{Tr} \Lambda \rho = 0$, and hence $\rho \in F$, contradicting the assumption that $F$ is a face of $S_1$. \hfill \Box

We summarize Theorems 8.1 and 8.2 as follows.

**Theorem 8.3.** There is a one to one correspondence between exposed faces of $S_1$ and exposed faces of $S^1_1$. The faces in each pair are dual (orthogonal) to each other.

Since the extremal points of $S_1$ are the pure product states, by Theorem 2.1 the extremal points of a face $F \in S_1$ are the pure product states contained in $F$. It follows that the extremal points of the face $\mathcal{Y}^\circ$ are the common zeros of all the witnesses in $\mathcal{Y}$. We have actually proved the following result.

**Theorem 8.4.** A set of product vectors in $\mathcal{H}$ is the complete set of zeros of some witness if and only if they are the extremal points of an exposed face of $S_1$ when regarded as states in $S_1$.

The remaining question, to which we do not know the answer, is whether $S_1$ has unexposed faces. We state the following theorem, which actually holds not only for $S_1$ but for any compact convex set.

**Theorem 8.5.** Every proper face of $S_1$ is contained in an exposed face of $S_1$.

*Proof.* Given a face $F$ of $S_1$, we have to prove that there exists a witness $\Omega$ such that $F$ is contained in the dual face $\Omega^\circ$.

Choose $\rho \in F$, in the interior of $F$ if $F$ contains more than one point. Choose also a separable state $\sigma \notin F$, and define $\tau = (1 + t)\rho - t\sigma$. Since $F$ is a face, and $\tau \in S_1$ for $-1 \leq t \leq 0$, we know that $\tau \notin S_1$ for every $t > 0$, and the set

$$\mathcal{Y}(t) = \{ \Lambda \in S^1_1 \mid \text{Tr} \Lambda \tau \leq 0 \} \quad (92)$$

is nonempty for every $t > 0$. Every $\mathcal{Y}(t)$ is a compact set, and $\mathcal{Y}(t_1) \subset \mathcal{Y}(t_2)$ for $0 < t_1 < t_2$. Hence, the intersection of all sets $\mathcal{Y}(t)$ for $t > 0$ is nonempty and contains at least one witness $\Omega$ such that $\text{Tr} \Omega \tau \leq 0$ for every $t > 0$. Clearly we must then have $\text{Tr} \Omega \rho = 0$. Since $\text{Tr} \Omega \rho = 0$ for one point $\rho$ in the interior of the face $F$, it follows that $\text{Tr} \Omega \rho = 0$ for every $\rho \in F$. \hfill \Box

Unfortunately, this does not amount to a proof that $F$ is exposed, because it might happen that $\text{Tr} \Omega \sigma = 0$ even though $\sigma \notin F$. 

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8.2 Faces of $\mathcal{D}_1$ and $\mathcal{P}_1$

When discussing faces of $\mathcal{S}_1$, the set of separable states, it may be illuminating to consider the simpler examples of faces of $\mathcal{D}_1$, the set of density matrices, and faces of $\mathcal{P}_1$, the set of PPT states. Recall that $\mathcal{D}_1$ is selfdual, $\mathcal{D}^\circ_1 = \mathcal{D}_1$. The fact that all faces of $\mathcal{D}_1$ and $\mathcal{P}_1$ are exposed may indicate that the same is true for all faces of $\mathcal{S}_1$.

A face $\mathcal{F}$ of $\mathcal{D}_1$ is a complete set of density matrices on a subspace $U \subset \mathcal{H}$, thus there is a one to one correspondence between faces of $\mathcal{D}_1$ and subspaces of $\mathcal{H}$. A density matrix $\rho$ belongs to the face $\mathcal{F}$ when $\text{Img} \rho \subset U$, and it is an interior point of $\mathcal{F}$ when $\text{Img} \rho = U$.

It is straightforward to show that when $\rho, \sigma \in \mathcal{D}_1$ we have $\text{Tr} \rho \sigma = 0$ if and only if $\text{Img} \rho \perp \text{Img} \sigma$. Hence, the dual, or opposite, face $\mathcal{F}^\circ$ is the set of density matrices on the subspace $U^\perp$, the orthogonal complement of $U$. The double dual of $\mathcal{F}$ is $\mathcal{F}$ itself, $\mathcal{F}^{\circ\circ} = \mathcal{F}$, since $(U^\perp)^\perp = U$.

Every proper face $\mathcal{F}$ of $\mathcal{D}_1$ is exposed, since it is the dual of an arbitrarily chosen interior point $\sigma \in \mathcal{F}^\circ$.

The definition $\mathcal{P}_1 = \mathcal{D}_1 \cap \mathcal{D}^\circ_1$ implies, by Theorem 2.2, that every face $\mathcal{G}$ of $\mathcal{P}_1$ is an intersection $\mathcal{G} = \mathcal{E} \cap \mathcal{F}^\circ$, where $\mathcal{E}$ and $\mathcal{F}$ are faces of $\mathcal{D}_1$. This is the geometrical meaning of the procedure for finding extremal PPT states introduced in [33].

It follows that every face of $\mathcal{P}_1$ is exposed. In fact, the face $\mathcal{G}$ is dual to a decomposable witness $\rho + \sigma^\circ P$ where $\rho, \sigma \in \mathcal{D}$, such that $\mathcal{E}$ is dual to $\rho$ and $\mathcal{F}$ is dual to $\sigma$.

8.3 Unexposed faces of $\mathcal{S}^\circ_1$

The Choi–Lam witness $\Omega_C$, as given in equation (72) with $\theta = 0$, $a = c = 1$, $b = 0$, is an example of an extremal witness, a zero dimensional face of $\mathcal{S}^\circ_1$, which is not exposed. The three isolated product vectors defined in equation (73) and the continuum of product vectors defined in equation (74), interpreted as states in $\mathcal{S}_1$, are the extremal points of the dual face $\mathcal{F}_C = \{\Omega_C\}^\circ \subset \mathcal{S}_1$. One may check both numerically and analytically that the face $\mathcal{F}_C$ has dimension 21. The separable states in the interior of $\mathcal{F}_C$ have rank seven, since they are constructed from product vectors in a seven dimensional subspace.

We find numerically that the constraints $U_0$ and $U_1$ associated with the zeros of $\Omega_C$ define a four dimensional face of $\mathcal{S}^\circ_1$. This is then the dual face $\mathcal{F}_C^\circ$, the double dual of $\Omega_C$. The last four constraints needed to prove that $\Omega_C$ is extremal come from the constraints $U_2$ and $U_3$ expressing the quartic nature of the zeros.

This is one example showing the mechanism for how faces of $\mathcal{S}^\circ_1$ may avoid being exposed. In general, a witness $\Omega$ having one or more isolated quartic zeros will be an interior point of an unexposed face. This unexposed face is then a face of a larger exposed face consisting of witnesses having the same zeros as $\Omega$, but such that all the isolated zeros are quadratic.

8.4 Simplex faces of $\mathcal{S}_1$

Theorem 8.4 expresses the relation between zeros of entanglement witnesses and exposed faces of $\mathcal{S}_1$, the set of separable states. We do not know whether $\mathcal{S}_1$ has unexposed faces. We consider first faces that are simplexes, having only a finite number of extremal points.
8.4.1 Faces of $S_1$ dual to quadratic extremal witnesses

The exposed faces of $S_1$ defined by extremal witnesses with only quadratic zeros are simplexes, and as such are particularly simple to study. Given the product vectors $\psi_i = \phi_i \otimes \chi_i$ for $i = 1, 2, \ldots, k$, with $k = n + 1$, as the zeros of a quadratic extremal witness $\Omega$. The corresponding product states $\rho_i = \psi_i \psi_i^\dagger$ are the vertices of an $n$-simplex, which is the exposed face $\Omega^o$ dual to $\Omega$.

Let $\rho$ be an interior point of this face,

$$\rho = \sum_{i=1}^{k} p_i \rho_i, \quad \sum_{i=0}^{k} p_i = 1, \quad p_i > 0.$$ (93)

According to Theorem 4.6, both $\rho$, constructed from the zeros $\phi_i \otimes \chi_i$, and its partial transpose $\rho^P$, constructed in the same way from the partially conjugated zeros $\phi_i \otimes \chi_i^*$, have full rank $N = N_a N_b$. Thus, $\rho$ lies not only in the interior of $\mathcal{D}_1$, the set of density matrices, but also in the interior of $\mathcal{P}_1$, the set of PPT states.

This geometric fact has the following interesting consequence. Let $\lambda$ denote the smallest one among the eigenvalues of $\rho$ and $\rho^P$, we know that $0 < \lambda < 1/N$. Then we may construct entangled PPT states from the separable state $\rho$ and the maximally mixed state $\rho_0$ as

$$\sigma = p\rho + (1-p)\rho_0, \quad 1 < p \leq \frac{1}{1 - N\lambda}. $$ (94)

The number of zeros of generic quadratic extremal witnesses presented in Table 1 has consequences also for the geometry of $S_1$. In dimensions $2 \times 4$ and $3 \times 3$ such a witness will have $N$ zeros and define a face of $S_1$ in the interior of $\mathcal{P}_1 \subset \mathcal{D}_1$. The boundary of this face will consist of other faces of $S_1$ defined by less than $N$ zeros, accordingly these faces are located inside faces of $\mathcal{D}_1$ on the boundary of $\mathcal{D}_1$. In higher dimensions such a witness has more than $N$ zeros, and defines a face of $S_1$ also in the interior of $\mathcal{D}_1$, but such that its boundary contains faces still in the interior of $\mathcal{D}_1$. In this way the geometry of $S_1$ in relation to $\mathcal{D}_1$ becomes more and more complicated as the dimensions increase.

8.4.2 Some numerical results

In an attempt to learn more about the geometry of simplex faces we have studied numerically in dimension $3 \times 3$ the faces of $S_1$ dual to generic quadratic extremal witnesses. They are 8-simplexes, each defined by 9 linearly independent pure product states that are the zeros of the witness. Our sample consisted of 169 extremal witnesses found in random numerical searches.

Volumes

Define the edge length factors $f_{ij} = d_{ij}^2 = \|\rho_i - \rho_j\|^2$ in the Hilbert–Schmidt norm, and the symmetric $(n+2) \times (n+2)$ Cayley–Menger matrix

$$D = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & f_{12} & \cdots & f_{1k} \\ 1 & f_{21} & 0 & \cdots & f_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & f_{k1} & f_{k2} & \cdots & 0 \end{pmatrix}. $$ (95)
Figure 5: Ratio of volumes $V^*$ and $V_{\text{reg}}$ of 8-simplex faces of $S_1$ in $3 \times 3$. $V^*$ is the simplex volume maximized under SL $\otimes$ SL transformations, and $V_{\text{reg}}$ is the volume of the regular simplex of orthogonal pure product states.

The volume of this $n$-simplex is then given by

$$V = \frac{\sqrt{|\det(D)|}}{2^n n!}.$$  \hspace{1cm} (96)

The volume of the regular $n$-simplex with edge length $s$ is

$$V_{\text{reg}} = \frac{s^n}{n!} \sqrt{\frac{n + 1}{2^n}}.$$ \hspace{1cm} (97)

The maximal distance between two pure states is $\sqrt{2}$, when the states are orthogonal. For $n = 8$ and $s = \sqrt{2}$ we have $V_{\text{reg}} = 3/8! = 7.440 \times 10^{-5}$.

Due to the highly irregular shapes we find volumes of the faces varying over five orders of magnitude. Since we regard density matrices related by SL $\otimes$ SL transformations as equivalent, a natural question is how regular these simplexes can be made by such transformations, in other words, what is the maximum volume $V^*$ we may obtain. Figure 5 shows our data for the ratio $V^*/V_{\text{reg}}$. There is some variation left in this ratio, indicating that the 8-simplexes are genuinely irregular.
Figure 6: Ratio of distances $d^*_c$ and $R_m$ for 8-simplex faces of $S_1$ in dimension $3 \times 3$. $d^*_c$ is the distance from the center of the face minimized under SL $\otimes$ SL transformations, and $R_m$ is the radius of the maximal ball of separable states. The points are plotted in the same order as in Figure 5.

**Positions relative to the maximally mixed state**

The second geometric property we have studied is the distance from the maximally mixed state to the centre of each simplex face, defined as the average of the vertices,

$$\rho_c = \frac{1}{k} \sum_{i=1}^{k} \rho_i.$$  (98)

We compare this distance to the radius of the maximal ball of separable states centered around the maximally mixed state [13],

$$R_m = \frac{1}{\sqrt{N(N-1)}}.$$  (99)

For $N = 3 \times 3$ we have $R_m = 1/\sqrt{72} = 0.1179$. The distance $d_c = \|\rho_c - \rho_0\|$ can be minimized by SL $\otimes$ SL transformations on $\rho_c$, resulting in a unique minimal distance $d^*_c$ for each equivalence class of faces. Figure 6 shows our data for the ratio $d^*_c/R_m$. We see that $d^*_c$ does not saturate the lower bound $R_m$, and this is another indication of the intrinsic irregularity of the 8-simplexes.

The third property studied is the orientation of each simplex relative to the maximally mixed state $\rho_0$. On a given face there exists a unique state $\rho_{\text{min}}$ closest to $\rho_0$, the minimum distance is $d_{\text{min}} = \|\rho_{\text{min}} - \rho_0\|$. In dimension $N = N_a N_b$ the distance from any pure state to
the maximally mixed state $\rho_0$ is $\sqrt{(N - 1)/N}$, and in our case this gives an upper limit

$$d_{\text{min}} < \sqrt{\frac{8}{9}} = 0.9428.$$  \hspace{1cm} (100)$$

With our sample of 180 faces it happens in only four cases, or 2\%, that $\rho_{\text{min}}$ lies in the interior of the face and has the full rank 9. In the remaining 98\% of the cases, $\rho_{\text{min}}$ lies on the boundary of the face and has lower rank.

Figure 7 shows the rank and distance for the state $\rho_{\text{min}}$ in each face in our sample. We see a tendency that the minimum distance $d_{\text{min}}$ is smaller when the rank of $\rho_{\text{min}}$ is higher. This confirms our expectation that the most regular simplex faces are positioned most symmetrically relative to the maximally mixed state, and also come closest to this state.

We find numerically that if we generate an 8-simplex by generating a random set of 9 pure product states, then $\rho_{\text{min}}$ will lie in the interior of the simplex and have full rank in about 90\% of the cases. Also we observe no ranks smaller than 6. Thus, Figure 7 proves that a simplex face generated by a random search for an extremal witness looks very different from a randomly generated simplex. A random set of product vectors that define an 8-simplex will in general not be the zeros of an entanglement witness, and the simplex will not be a face of $S_1$. 

Figure 7: The rank of $\rho_{\text{min}}$ and its distance $d_{\text{min}}$ from the maximally mixed state for 8-simplex faces in dimension $3 \times 3$. The faces are derived from our set of quadratic extremal entanglement witnesses found in random searches using Algorithm 1.
8.5 Other types of faces of $S_1$

To every entanglement witness there corresponds an exposed face of $S_1$, and the great variety of entanglement witnesses implies a similar variety of faces of $S_1$. The class of simplex faces, having only a finite number of extremal points, is rather special, other faces may have only continuous sets of extremal points, or both discrete and continuous subsets of extremal points. Some special examples in dimension $3 \times 3$ may serve as illustrations.

The Choi–Lam witness is a good example. It has three discrete zeros and one continuous set of zeros, and these zeros in their role as pure product states are the extremal points of a face of $S_1$.

An extremal decomposable witness, i.e. a pure state or the partial transpose of a pure state, defines a face of $S_1$ with one single continuous set of extremal points. To be more specific, consider a pure state $\Omega = \psi \psi^\dagger$, then the zeros of $\Omega$ are the product vectors orthogonal to $\psi$.

We consider two typical cases.

One example is the product vector $\psi = e_1 \otimes e_1$. Then the zeros are the product vectors

$$\phi \otimes \chi = (a_1 e_1 + a_2 e_2 + a_3 e_3) \otimes (b_1 e_1 + b_2 e_2 + b_3 e_3)$$

with either $a_1 = 0$ or $b_1 = 0$. These product vectors produce pure product states belonging to a full matrix algebra in dimension $2 \times 3$ if $a_1 = 0$, and in dimension $3 \times 2$ if $b_1 = 0$. They are the extremal points of a face of the type called in [16] a convex combination of matrix algebras.

Another example is the Bell type entangled pure state

$$\psi = \frac{1}{\sqrt{3}} (e_1 \otimes e_1 + e_2 \otimes e_2 + e_3 \otimes e_3).$$

The zeros in this case are the product vectors as in equation (101) with

$$a_1 b_1 + a_2 b_2 + a_3 b_3 = 0.$$  \hspace{1cm} (103)

For every vector $\phi = a_1 e_1 + a_2 e_2 + a_3 e_3$ there is a two dimensional subspace of vectors $\chi = b_1 e_1 + b_2 e_2 + b_3 e_3$ satisfying this orthogonality condition. And vice versa, for every vector $\chi$ there is a two dimensional subspace of vectors $\phi$. These pure product states are the extremal points of a face which is neither a simplex nor a convex combination of matrix algebras.

8.6 Minimal convex decomposition

We know that any point in a compact convex set may be written as a convex combination of extremal points, but if we want to do the decomposition in practice an important question is how many extremal points we need. We would like to know a minimal number of extremal points that is sufficient for all points. The facial structure of the set is then relevant.

The theorem of Carathéodory gives a sufficient number of extremal points as $n + 1$ where $n$ is the dimension of the set [39]. However, the set $D_1$ of normalized density matrices is an example where one can do much better. The dimension of the set is $n = N^2 - 1$, where $N$ is the dimension of the Hilbert space, but the spectral representation of a density matrix in terms of its eigenvalues and eigenvectors is a decomposition using only $N$ extremal points. In order to see how this number $N$ is related to the facial structure of $D_1$, consider the following proof of Carathéodory’s theorem.
Any point \( x \) in a compact convex set \( C \) is either extremal or an interior point of a unique face \( F_1 \), which might be the whole set \( C \). If \( x \) is not extremal it may be written as a convex combination

\[
x = (1 - p_1)x_1 + p_1y_1 ,
\]

(104)

where \( x_1 \) is an arbitrary extremal point of \( F_1 \) and \( y_1 \) is another boundary point of \( F_1 \). If \( y_1 \) is extremal we define \( x_2 = y_1 \), otherwise \( y_1 \) is an interior point of a proper face \( F_2 \) of \( F_1 \), and we write

\[
y_1 = (1 - p_2)x_2 + p_2y_2 ,
\]

(105)

where \( x_2 \) is an extremal point of \( F_2 \) and \( y_2 \) is a boundary point of \( F_2 \). Continuing this process we obtain a decomposition of \( x \) as a convex combination of extremal points \( x_1, x_2, \ldots, x_k \in C \), and a sequence \( F_1 \supset F_2 \supset \ldots \supset F_k \) of faces of decreasing dimensions

\[
n \geq n_1 > n_2 > \ldots > n_k = 0 .
\]

(106)

The length of the sequence is \( k \), and the obvious inequality \( k \leq n + 1 \) is Carathéodory’s theorem.

For the set \( D_1 \) of normalized density matrices the longest possible sequence of face dimensions has length \( N \), it is

\[
N^2 - 1 > (N-1)^2 - 1 > \ldots > (N-j)^2 - 1 > \ldots > 8 > 3 > 0 .
\]

(107)

In general, we decompose an arbitrary density matrix \( \rho \) of rank \( r \) as a convex combination of \( r \) pure states that may be eigenvectors of \( \rho \), but need not be.

We may apply this procedure to the decomposition of an arbitrary separable state as a convex combination of pure product states. As we see, the number of pure product states we have to use depends very much on the facial structure of the set of separable states. It might happen, for example, that the face \( F_2 \) is the dual of a quadratic witness, and then it contains only a finite number of pure product states, much smaller than the dimension \( N^2 - 1 \) of the set \( S_1 \) of normalized separable states. Recall that the pure product states in such a face are the zeros of the witness, and the number of zeros is largest when the witness is extremal. In the generic case the number of zeros of a quadratic extremal witness is \( n_c \), as given by equation (43) and tabulated in Table 1.

It seems likely therefore that also in the decomposition of separable states one could do much better than the \( N^2 \) pure product states guaranteed by Carathéodory’s theorem. We consider this an interesting open problem for further study.

### 9 Optimal and extremal witnesses

The notion of optimal entanglement witnesses was developed by Lewenstein et al. [26, 29]. In this section we comment briefly on the relation between optimal and extremal witnesses. In systems of dimension \( 2 \times N_b \) and \( 3 \times 3 \) the two concepts are, at least generically, closely related. This has significant geometric consequences.

Recall the definition that a witness \( \Omega \) is extremal if and only if there does not exist two other witnesses \( \Omega_0 \) and \( \Omega_1 \) such that

\[
\Omega = (1 - p)\Omega_0 + p\Omega_1 , \quad 0 < p < 1 .
\]

(108)
Lewenstein et al. introduce two different concepts of optimality and give two necessary and sufficient conditions for optimality, similar to the condition for extremality [26]. By their Theorem 1, a witness $\Omega$ is optimal if and only if it is not a convex combination of this form where $\Omega_1$ is a positive semidefinite matrix. By their Theorem 1(b), $\Omega$ is nondecomposable optimal if and only if it is not a convex combination of this form where $\Omega_1$ is a decomposable witness. Obviously, extremal witnesses are optimal by both optimality criteria.

Ha and Kye give examples to show that an optimal witness which is nondecomposable need not be nondecomposable optimal according to the definition of Lewenstein et al., hence they propose to replace the ambiguous term “nondecomposable optimal witness” by “optimal PPTES witness”, where PPTES refers to entangled states with positive partial transpose [57]. Here we will use the original terminology.

Note that the criterion for optimality is not invariant under partial transposition, hence a witness $\Omega$ may be optimal while its partial transpose $\Omega^P$ is not optimal, and vice versa. The criterion for nondecomposable optimality, on the other hand, is invariant under partial transposition, so that $\Omega$ is nondecomposable optimal if and only if $\Omega^P$ is nondecomposable optimal.

Apparently the condition of being extremal is stricter than those of being optimal or nondecomposable optimal. Accordingly there should, in general, exist plenty of nonextremal witnesses that are either optimal or nondecomposable optimal. We now investigate this question further in the spirit of Theorem 4.6. We can immediately give sufficient optimality conditions.

**Theorem 9.1.** A witness $\Omega$ is optimal if its zeros span the Hilbert space.

$\Omega$ is nondecomposable optimal if its zeros span the Hilbert space, and at the same time its partially conjugated zeros span the Hilbert space.

*Proof.* Equation (108) implies that the zeros and Hessian zeros of $\Omega$ are also zeros and Hessian zeros of $\Omega_0$ and $\Omega_1$. But if $\Omega_1$ is positive semidefinite and its zeros span the Hilbert space, then $\Omega_1 = 0$. Similarly, if $\Omega_1$ is decomposable and its zeros and partially conjugated zeros both span the Hilbert space, then $\Omega_1 = 0$.

For a quadratic witness these conditions are not only sufficient but also necessary.

**Theorem 9.2.** Let $\Omega$ be a quadratic witness.

Then $\Omega$ is optimal if and only if its zeros span the Hilbert space.

$\Omega$ is nondecomposable optimal if and only if its zeros span the Hilbert space and its partially conjugated zeros also span the Hilbert space.

Hence, by Theorem 5.1, if $\Omega$ is nondecomposable optimal it is nondecomposable.

*Proof.* We have to prove the “only if” part, and we reason like in the proofs of Theorem 4.6 and Theorem 4.3. If the zeros do not span the Hilbert space, there exists a vector $\psi$ orthogonal to all zeros, and we define $\Omega_1 = \psi\psi^\dagger$. Then the zeros of $\Omega_1$ include the zeros of $\Omega$, and we know that $\Omega_1 \neq \Omega$ because $\Omega$ is quadratic and $\Omega_1$ is quartic. The line segment from $\Omega_1$ to $\Omega$ consists of witnesses having exactly the same zeros and Hessian zeros as $\Omega$ ($\Omega$ has no Hessian zeros since it is quadratic). By Theorem 4.2 this line segment can be prolonged within $S_{\Omega}^\circ$ so that it gets $\Omega$ as an interior point. Hence $\Omega$ is neither optimal nor nondecomposable optimal.

If the partially conjugated zeros do not span the Hilbert space, then there exists a vector $\eta$ orthogonal to all the partially conjugated zeros. Now we define $\Omega_1 = (\eta\eta^\dagger)^P$, and use it in the same way as a counterexample to prove that $\Omega$ is not nondecomposable optimal. 

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In dimensions $3 \times 3$ and $2 \times N_b$, a witness $\Omega$ with doubly spanning zeros will generically be extremal, according to Table 1. We expect, however, that the construction described in Subsection 6.3.3 will lead to nongeneric counterexamples in these dimensions (although we have not checked this explicitly). We state the following theorem.

**Theorem 9.3.** In dimensions $2 \times N_b$ and $3 \times 3$ a generic witness with only quadratic zeros is nondecomposable optimal if and only if it is extremal.

Since we do not have a complete understanding of constraints from quartic zeros, we leave the relation between nondecomposable optimality and extremality of quartic witnesses as an open problem.

From Table 1 we understand that in higher dimensions the number of zeros of a quadratic extremal witness must be larger than the Hilbert space dimension $N = N_a \times N_b$. Hence nonextremal witnesses with doubly spanning zeros must be very common, so that nondecomposable optimality is a significantly weaker property than extremality. In particular, when we search for generic quadratic extremal witnesses and reach the stage where the witnesses have $N$ or more zeros, then every face of $S^T_1$ we encounter will consist entirely of nondecomposable optimal witnesses, most of which are not extremal.

The observations made above give a picture of increasingly complicated geometry as dimensions increase. In dimensions $2 \times 2$ and $2 \times 3$ every witness is decomposable [11, 14]. In $2 \times N_b$ and $3 \times 3$ a generic quadratic witness is either nondecomposable optimal and extremal, or it is neither. In higher dimensions there exist an abundance of nondecomposable optimal nonextremal witnesses.

**10 The SPA separability conjecture**

In this section we comment briefly on the conjecture put forward by Korbicz et al. that what they and others define as the structural physical approximation (the SPA) of an optimal entanglement witness is always a separable density matrix [31]. This conjecture was supported by several explicit constructions [54, 58, 59]. Nevertheless it can not be true as stated, for the simple reason that the SPA of a randomly chosen nondecomposable optimal witness has only about fifty per cent chance of being a PPT state, which is a minimum requirement for its being separable. This was pointed out recently by Ha and Kye [32]. The SPA of a positive map was defined more generally by Horodecki and Ekert [30].

An obvious modification of the conjecture would be to redefine the SPA as the nearest PPT matrix instead of the nearest positive matrix. Recent counterexamples disprove even this modified separability conjecture [32, 40]. We point out here that these counterexamples are not generic, and we have made a small numerical investigation of how the modified conjecture works for generic quadratic extremal (and hence optimal) witnesses. We are unable to draw a definitive conclusion because of the limited numerical precision of our separability test.

Given a state $\rho$ on the Hilbert space $\mathcal{H}_a \otimes \mathcal{H}_b$. If $\rho$ is entangled there exists a witness $\Omega$ detecting the entanglement by the negativity of the expectation value $\text{Tr} \, \Omega \rho$. A more sophisticated detection scheme for entanglement is to use the witness $\Omega$ in order to define a map transforming the state to be tested for entanglement, rather than using $\Omega$ directly as an observable to be measured. This is where the need arises for approximating $\Omega$ by a positive matrix called the SPA of $\Omega$. 

There are several ways to define a one to one correspondence between entanglement witnesses and positive maps. Following [11], we associate the witness $\Omega$ with the map

$$M_\Omega = L_{\Omega \Omega^TP} : H_b \to H_a,$$

(109)

where $L_A^\dagger$ is defined in equation (10), and $\Omega^{TP}$ is the partial transpose of $\Omega$ with respect to subsystem $a$. Let $I_a$ be the identity map on $H_a$, and write

$$\sigma = (I_a \otimes M_\Omega) \rho,$$

(110)

with $\rho \in H_a \otimes H_b$ and $\sigma \in H_a \otimes H_a$. Explicitly in terms of matrix elements this reads

$$\sigma_{ij;kl} = \sum_{m,n} \Omega_{lm;jn} \rho_{in;km}.$$  

(111)

Introducing an unnormalized maximally entangled pure state

$$\psi = \sum_i e_i \otimes e_i \in H_a \otimes H_a$$

(112)

we now have that

$$\psi^\dagger \sigma \psi = \sum_{i,k} \sigma_{ii;kk} = \sum_{i,k,m,n} \Omega_{km;in} \rho_{in;km} = \text{Tr} \Omega \rho.$$  

(113)

If $\rho$ is separable then obviously $\sigma$ is positive, since $M_\Omega$ is a positive map. And conversely, if $\rho$ is entangled we may always choose $\Omega$ such that $\text{Tr} \Omega \rho < 0$, then $\sigma$ is not positive, by equation (113). In this way the map $M_\Omega$ provides a separability test for $\rho$, based on the property of $M_\Omega$ that it is positive but not completely positive, so that $I_a \otimes M_\Omega$ is not a positive map.

A mathematical map $I_a \otimes M_\Omega$ mapping a physical state $\rho$ outside the set of physical states does not represent a physical process. When we want a physical map, the SPA approach is to mix in the unit matrix $I$ and replace $\Omega$ by

$$\Sigma(p) = (1-p)\Omega + \frac{p}{N} I,$$

(114)

choosing a value of $p$, $0 < p < 1$, such that $\Sigma(p)$ is a positive matrix. Then the corresponding map $M_{\Sigma(p)}$ is completely positive. Three special values of $p$ are of particular interest. Let

- $p_0$ be the smallest value of $p$ such that $\Sigma(p)$ is a separable density matrix;
- $p_1$ be the smallest value of $p$ such that $\Sigma(p)$ is a density matrix;
- $p_2$ be the smallest value of $p$ such that $(\Sigma(p))^P$ is a density matrix.

If $\lambda_1 < 0$ and $\lambda_2 < 0$ are the lowest eigenvalues of $\Omega$ and $\Omega^P$, respectively, then

$$p_1 = -\frac{N\lambda_1}{1-N\lambda_1}, \quad p_2 = -\frac{N\lambda_2}{1-N\lambda_2}.$$  

(115)

The SPA of $\Omega$ is defined in [31] as $\tilde{\Omega} = \Sigma(p_1)$. Define

$$\tilde{\sigma} = (I_a \otimes M_{\tilde{\Omega}}) \rho = (1-p_1) \sigma + \frac{p_1}{N} ((\text{Tr}_b \rho) \otimes I_b).$$  

(116)
This matrix has only nonnegative eigenvalues, by construction, but we might use it to check whether $\sigma$ has negative eigenvalues.

Clearly $p_0 \geq p_1$ and $p_0 \geq p_2$, but we may have either $p_1 < p_2$, $p_1 = p_2$, or $p_1 > p_2$. The SPA of $\Omega$ is a PPT state if and only if $p_1 \geq p_2$. It follows directly from the definitions that the SPA of the witness $\Omega^P$ is $(\Sigma(p_2))^P$, and this is a PPT state if and only if $p_2 \geq p_1$.

When we find an extremal witness $\Omega$ in a random numerical search by Algorithm 1, presumably the probabilities of finding $\Omega$ and $\Omega^P$ are equal. Hence we expect to have about fifty per cent probability of finding an extremal witness with an SPA which is a PPT state. This is also what we see in practice.

For each extremal witness $\Omega$ found in dimensions $3 \times 3$ and $3 \times 4$ we have computed the SPA of $\Omega$ and of $\Omega^P$. As expected, in each case one SPA is a PPT state and the other one is not. The number of PPT states found originating from $\Omega$ or from $\Omega^P$ is listed in Table 4.

|       | $3 \times 3$ | $3 \times 4$ |
|-------|--------------|--------------|
| $\Omega$ | 81           | 41           |
| $\Omega^P$ | 90           | 24           |

Table 4: Number of cases where the SPA of $\Omega$ or $\Omega^P$ is a PPT state, when $\Omega$ is a quadratic extremal witness found numerically in dimension $3 \times 3$ or $3 \times 4$.

The question whether the SPA $\bar{\Omega}$ of a witness $\Omega$ is a separable state is interesting because separability simplifies the physical implementation of the map $M_{\bar{\Omega}}$. Since the original separability conjecture of Korbicz et al. fails, a natural question is whether the SPA is always separable when it is a PPT state. Again there are counterexamples, as mentioned [32, 40]. On the other hand, these counterexamples are rather special, and there remains a possibility that the SPA of a generic extremal witness with only quadratic zeros could be separable if it is a PPT state.

For this reason, in our numerical examples we have tried to check the separability of the SPA whenever it is a PPT state. We find that it is always very close to being separable, in no case are we able to conclude that it is certainly not separable. Unfortunately, our numerical separability test is not sufficiently precise that we may state with any conviction the opposite conclusion that the state is separable.

In conclusion, we do not know to what extent a modified SPA separability conjecture holds, which excludes the states that are not PPT states. On the other hand, if we regard separability as an essential property of the SPA, it seems that the natural solution would be to define the SPA by the parameter value $p = p_0$, where $\Sigma(p)$ first becomes separable, rather than by the value $p = p_1$, where $\Sigma(p)$ first becomes positive.

11 A real problem in a complex cloak

We want to outline here a different approach to the problem of describing the convex cone $S^\circ$ of entanglement witnesses, where we regard it as a real rather than a complex problem. This means that we treat $S^\circ_1$ as a subset of a higher dimensional compact convex set. We are motivated by the observation that the problem is intrinsically real, since $H$ is a real vector space, $f_\Omega$ is a real valued function, and some of the constraints discussed in Section 3 are explicitly real. In particular, the second derivative matrix, the Hessian, defining constraints at a quartic zero of a witness is a real and not a complex matrix.
Another motivation is the possibility of expressing the extremal points of $S^1_\circ$ as convex combinations of extremal points of the larger set. As an example we show how a pure state as a witness is a convex combination of real witnesses that are not of the complex form.

In order to arrive at an explicitly real formulation of the problem we proceed as follows. Define $J: \mathbb{R}^{2N_a} \to \mathbb{C}^{N_a}$ and $K: \mathbb{R}^{2N_b} \to \mathbb{C}^{N_b}$ as

$$J = (I_a, iI_a), \quad K = (I_b, iI_b),$$

and define

$$Z = (J \otimes K)^\dagger \Omega (J \otimes K).$$

Then if $\phi = Jx$ and $\chi = Ky$ we have that

$$g_Z(x, y) = (x \otimes y)^\dagger Z(x \otimes y) = (\phi \otimes \chi)^\dagger \Omega (\phi \otimes \chi) = f_\Omega (\phi, \chi).$$

Since $Z$ is a Hermitian matrix, its real part is symmetric and its imaginary part antisymmetric. The expectation value $g_W(x, y)$ is real because only the symmetric part of $Z$ contributes. Furthermore, only the part of $Z$ that is symmetric under partial transposition contributes. Hence $g_Z(x, y) = g_W(x, y)$ when we define

$$W = \frac{1}{2} \text{Re}(Z + Z^p).$$

Since $J \otimes K = (I_a \otimes K, iI_a \otimes K)$ is an $N \times (4N)$ matrix, $Z$ is a $(4N) \times (4N)$ matrix,

$$Z = \begin{pmatrix} X & iX \\ -iX & X \end{pmatrix},$$

where $X$ is a $(2N) \times (2N)$ matrix,

$$X = (I_a \otimes K)^\dagger \Omega (I_a \otimes K).$$

The partial transposition of $Z$ transposes submatrices of size $(2N_b) \times (2N_b)$.

We may now replace the complex biquadratic form $f_\Omega$ by the real form $g_W$, and repeat the analysis in Section 3 almost unchanged. We therefore see that complex witnesses in dimension $N_a \times N_b = N$ correspond naturally to real witnesses in $(2N_a) \times (2N_b) = 4N$.

Write the matrix elements of $\Omega$ as

$$(\Omega_{ik})_{jl} = \Omega_{ij,kl},$$

In this notation, $\Omega_{ik}$ is an $N_b \times N_b$ submatrix of the $N \times N$ matrix $\Omega$. Then we have that

$$X_{ik} = K^\dagger \Omega_{ik} K = \begin{pmatrix} \Omega_{ik} & i\Omega_{ik} \\ -i\Omega_{ik} & \Omega_{ik} \end{pmatrix},$$

The complex matrix $\Omega_{ik}$ may always be decomposed as

$$\Omega_{ik} = A_{ik} + B_{ik} + i(C_{ik} + D_{ik}),$$

where $A_{ik}, B_{ik}, C_{ik}, D_{ik}$ are real matrices, and $A_{ik}, C_{ik}$ are symmetric, $B_{ik}, D_{ik}$ are antisymmetric. The Hermiticity of $\Omega$ means that

$$\Omega_{ik} = (\Omega_{ki})^\dagger = A_{ki} - B_{ki} - i(C_{ki} - D_{ki}),$$

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or equivalently,

\[ A_{ki} = A_{ik}, \quad B_{ki} = -B_{ik}, \quad C_{ki} = -C_{ik}, \quad D_{ki} = D_{ik}. \]  \hfill (127)

In particular,

\[ B_{ii} = C_{ii} = 0. \]  \hfill (128)

We finally arrive at the following explicit relation between the complex witness \( \Omega \) and the real witness \( W \),

\[ W = \begin{pmatrix} U & -V \\ V & U \end{pmatrix}, \]  \hfill (129)

with

\[ U_{ik} = \frac{1}{2} \text{Re}(X_{ik} + X_{ik}^\top) = \begin{pmatrix} A_{ik} & -D_{ik} \\ D_{ik} & A_{ik} \end{pmatrix}, \]

\[ V_{ik} = \frac{1}{2} \text{Im}(X_{ik} + X_{ik}^\top) = \begin{pmatrix} C_{ik} & B_{ik} \\ -B_{ik} & C_{ik} \end{pmatrix}. \]  \hfill (130)

Note that the \((2N_b) \times (2N_b)\) matrices \( U_{ik} \) and \( V_{ik} \) are symmetric by construction, \( U_{ik} = (U_{ik})^\top \) and \( V_{ik} = (V_{ik})^\top \). This means that \( W \) is symmetric under partial transposition, \( W^P = W \).

It also follows from the equations (130) and (127) that \( U_{ki} = U_{ik} \) and \( V_{ki} = -V_{ik} \). This means that the \((2N) \times (2N)\) matrix \( U \) is symmetric, \( U^\top = U \) because

\[ (U^\top)_{ik} = (U_{ki})^\top = U_{ki} = U_{ik}, \]  \hfill (131)

whereas \( V \) is antisymmetric, \( V^\top = -V \) because

\[ (V^\top)_{ik} = (V_{ki})^\top = V_{ki} = -V_{ik}. \]  \hfill (132)

This means that \( W \) is symmetric, \( W^\top = W \).

### 11.1 A pure state as a witness

If \( \Omega \) is a pure state, \( \Omega = \psi\psi^\dagger \) with \( \psi^\dagger \psi = 1 \), then

\[ f_\Omega(\phi, \chi) = (\phi \otimes \chi)^\dagger \Omega(\phi \otimes \chi) = |z|^2 = (\text{Re } z)^2 + (\text{Im } z)^2, \]  \hfill (133)

with

\[ z = (\phi \otimes \chi)^\dagger \psi = (x \otimes y)^\top (J \otimes K)^\dagger \psi. \]  \hfill (134)

We have seen that \( \Omega \) is extremal in \( S_1^0 \), but we see now that it is not extremal in the larger set of real witnesses that are not of the complex form given in equation (129).

Write \( \psi = a + ib \) with \( a, b \) real, and

\[ p = (J \otimes K)^\dagger \psi = \begin{pmatrix} q \\ -i\bar{q} \end{pmatrix}, \]  \hfill (135)

with

\[ q = (I_a \otimes K)^\dagger \psi. \]  \hfill (136)
Here $q$ is a $(2N) \times 1$ matrix, and if we write $q_i$ with $i = 1, 2, \ldots, N_a$ for the submatrices of size $(2N_b) \times 1$, we have that
\[
q_i = K^\dagger \psi_i = \begin{pmatrix} \psi_i^\dagger \\ -i \psi_i \end{pmatrix} = \begin{pmatrix} a_i + ib_i \\ b_i - ia_i \end{pmatrix} = r_i + i s_i, \tag{137}
\]
with
\[
\begin{align*}
  r_i &= \begin{pmatrix} a_i \\ b_i \end{pmatrix}, \\
  s_i &= \begin{pmatrix} b_i \\ -a_i \end{pmatrix}.
\end{align*} \tag{138}
\]

We now have that
\[
(\text{Re } z)^2 = (x \otimes y)^\dagger Z_r (x \otimes y), \quad (\text{Im } z)^2 = (x \otimes y)^\dagger Z_i (x \otimes y),
\]
with
\[
\begin{align*}
  Z_r &= (\text{Re } p)(\text{Re } p)^\dagger = \begin{pmatrix} r r^\dagger & r s^\dagger \\ s r^\dagger & s s^\dagger \end{pmatrix}, \\
  Z_i &= (\text{Im } p)(\text{Im } p)^\dagger = \begin{pmatrix} s s^\dagger & -r s^\dagger \\ -r s^\dagger & r r^\dagger \end{pmatrix}. \tag{140}
\end{align*}
\]

These two matrices are symmetric, $Z_r^\dagger = Z_r$ and $Z_i^\dagger = Z_i$, but we should also make them symmetric under partial transposition. Therefore we replace them by the matrices
\[
\begin{align*}
  W_r &= \frac{1}{2} (Z_r + Z_r^P) = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \\
  W_i &= \frac{1}{2} (Z_i + Z_i^P) = \begin{pmatrix} D & -C \\ -B & A \end{pmatrix}, \tag{141}
\end{align*}
\]
where
\[
\begin{align*}
  A_{ik} &= \frac{1}{2} (r_i r_k^\dagger + r_k r_i^\dagger) = \frac{1}{2} \begin{pmatrix} a_i a_k^\dagger + a_k a_i^\dagger \\ b_i b_k^\dagger + b_k b_i^\dagger \\ a_i b_k^\dagger + a_k b_i^\dagger \\ b_i a_k^\dagger + b_k a_i^\dagger \end{pmatrix}, \\
  B_{ik} &= \frac{1}{2} (r_i s_k^\dagger + s_k r_i^\dagger) = \frac{1}{2} \begin{pmatrix} a_i b_k^\dagger + a_k b_i^\dagger \\ b_i a_k^\dagger + b_k a_i^\dagger \\ -a_i a_k^\dagger + a_k a_i^\dagger \\ -b_i b_k^\dagger + b_k b_i^\dagger \end{pmatrix}, \tag{142} \\
  C_{ik} &= \frac{1}{2} (s_i r_k^\dagger + r_k s_i^\dagger) = \frac{1}{2} \begin{pmatrix} -a_i a_k^\dagger + a_k a_i^\dagger \\ b_i b_k^\dagger + b_k b_i^\dagger \\ -a_i b_k^\dagger + a_k b_i^\dagger \\ -b_i a_k^\dagger + b_k a_i^\dagger \end{pmatrix}, \\
  D_{ik} &= \frac{1}{2} (s_i s_k^\dagger + s_k s_i^\dagger) = \frac{1}{2} \begin{pmatrix} -b_i b_k^\dagger + b_k b_i^\dagger \\ -a_i b_k^\dagger + a_k b_i^\dagger \\ a_i a_k^\dagger + a_k a_i^\dagger \\ -a_i a_k^\dagger - a_k a_i^\dagger \end{pmatrix}.
\end{align*}
\]

12 Summary and outlook

In this article we have approached the problem of distinguishing entangled quantum states from separable states through the related problem of classifying and understanding entanglement witnesses. We have studied in particular the extremal entanglement witnesses from which all other witnesses may be constructed. We give necessary and sufficient conditions for a witness to be extremal, in terms of the zeros and Hessian zeros of the witness, and in terms of linear constraints on the witness imposed by the existence of zeros. The extremality conditions lead to systematic methods for constructing numerical examples of extremal witnesses.
We find that the distinction between quadratic and quartic zeros is all important when we classify extremal witnesses. Nearly all extremal witnesses found in random searches are quadratic, having only quadratic zeros. There is a minimum number of zeros a quadratic witness must have in order to be extremal, and most of the quadratic extremal witnesses have this minimum number of zeros. To our knowledge, extremal witnesses of this type have never been observed before, even though they are by far the most common.

The number of zeros of a quadratic extremal witness increases faster than the Hilbert space dimension. Since a witness is optimal if its zeros span the Hilbert space, this implies that in all but the lowest dimensions witnesses may be optimal and yet be very far from extremal.

The facial structures of the convex set of separable states and the convex set of witnesses are closely related. The zeros of a witness, whether quadratic or quartic, always define an exposed face of the set of separable states. The other way around, an exposed face of the set of separable states is defined by a set of pure product states that are the zeros of some witness, in fact, they are the common zeros of all the witnesses in a face of the set of witnesses. The existence of witnesses with quartic zeros is the root of the existence of nonexposed faces of the set of witnesses. It is unknown to us whether the set of separable states has unexposed faces.

One possible way to test whether or not a given state is separable is to try to decompose it as a convex combination of pure product states. In such a test it is of great practical importance to know the number of pure product states that is needed in the worst case. The general theorem of Carathéodory provides a limit of $n + 1$ where $n$ is the dimension of the set, but this is a rather large number, and an interesting unsolved problem is to improve this limit, if possible. We point out that this is a question closely related to the facial structure of the set of separable states, which in turn is related to the set of entanglement witnesses.

Another unsolved problem we may mention here again is the following. We have found a procedure for constructing an extremal witness from its zeros and Hessian zeros, but an arbitrarily chosen set of zeros and Hessian zeros does not in general define an extremal entanglement witness. How do we construct an extremal witness by choosing a set of zeros and Hessian zeros we want it to have? Clearly this is a much more complicated problem than the trivial problem of constructing a polynomial in one variable from its zeros.

In conclusion, by studying the extremal entanglement witnesses we have made some small progress towards understanding the convex sets of witnesses and separable mixed states. But this has also made the complexity of the problem even more clear than it was before. The main complication is the fact that zeros of extremal witnesses may be quartic, since this opens up an almost unlimited range of variability among the quartic witnesses. A full understanding of this variability seems a very distant goal. Nevertheless we believe that it is useful to pursue the study of extremal witnesses in order to learn more about the geometry of the set of separable states, and it is rather clear that a combination of analytical and numerical methods will be needed also in future work.

A Explicit expressions for constraints

Given a zero $(\phi_0, \chi_0)$, let $j_m$ for $m = 1, \ldots, 2(N_a - 1)$ be the column vectors of the matrix $J_0$. We construct them for example from an orthonormal basis $\phi_0, \phi_1, \ldots, \phi_{N_a-1}$ of $\mathcal{H}_a$, taking $j_{2l-1} = \phi_l, j_{2l} = i\phi_l$ for $l = 1, \ldots, N_a - 1$. Similarly, let $k_n$ for $n = 1, \ldots, 2(N_b - 1)$ be the column vectors of $K_0$. 53
Then the equations $T_0 \Omega = 0$, $T_1 \Omega = 0$ may be written as

$$
\begin{align*}
\text{Tr}(E^0 \Omega) &= 0, & E^0_i &= \phi_0 \phi_i^\dagger \otimes \chi_0 \chi_0^\dagger, \\
\text{Tr}(E^1 \Omega) &= 0, & E^1_i &= (j_m \phi_0^\dagger + \phi_0 j_m^\dagger) \otimes \chi_0 \chi_0^\dagger, \\
\text{Tr}(E^2 \Omega) &= 0, & E^2_i &= \phi_0 \phi_0^\dagger \otimes (k_n \chi_0^\dagger + \chi_0 k_n^\dagger).
\end{align*}
$$

(143)

With $z_i \in \text{Ker} G \Omega z_i^\dagger = (x_i^\dagger, y_i^\dagger)$ and $\xi_i = J_0 x_i$, $\zeta_i = K_0 y_i$, for $i = 1, \ldots, K$, the constraints $(T_2 \Omega)_i = 0$ given in equation (31) may be written explicitly as follows,

$$
\begin{align*}
\text{Tr}(F^1_{im} \Omega) &= 0, & F^1_{im} &= (\xi_i j_m^\dagger + j_m \xi_i^\dagger) \otimes \chi_0 \chi_0^\dagger + (\phi_0 j_m^\dagger + j_m \phi_0^\dagger) \otimes (\zeta_i \chi_0^\dagger + \chi_0 \zeta_i^\dagger), \\
\text{Tr}(F^2_{im} \Omega) &= 0, & F^2_{im} &= \phi_0 \phi_0^\dagger \otimes (\xi_i k_n^\dagger + k_n \xi_i^\dagger) + (\zeta_i \phi_0^\dagger + \phi_0 \zeta_i^\dagger) \otimes (\chi_0 k_n^\dagger + k_n \chi_0^\dagger).
\end{align*}
$$

(144)

System $T_3$ can be written as follows. For any linear combinations

$$
\xi = \sum_{i=1}^{K} a_i \xi_i, \quad \zeta = \sum_{i=1}^{K} a_i \zeta_i,
$$

(145)

\[ a_i \] with real coefficients $a_i$ and $\xi_i, \zeta_i$ as above, we have

$$
\text{Tr} G \Omega = 0, \quad G = (\xi \phi_0^\dagger + \phi_0 \xi^\dagger) \otimes \zeta \zeta^\dagger + \xi \zeta \zeta^\dagger \otimes (\zeta \chi_0^\dagger + \chi_0 \zeta^\dagger).
$$

(146)

This is one single constraint for each set of coefficients $a_i$. The minimum number of different linear combinations that we have to use is given by the binomial coefficient

$$
\binom{K+2}{3} = \frac{K(K+1)(K+2)}{6}.
$$

B Numerical implementation of Algorithm 1

B.1 Solving the optimization problem

In this section we describe some possibilities for solving the optimization problem (15). This question has received little attention in the physics community, and in the optimization literature focus shifted towards a rigorous rather than towards an “applied” approach. Two comments are in place. In [60] and [34] simple algorithms were presented which in our experience work fine in most situations. However, when applied to Algorithm 1 we repeatedly observe poor convergence, presumably due to degeneracies of eigenvalues. In [61] it is stated that a straightforward parametrization of problem (15) can not be solved in an efficient manner. Instead they present a formalism which again, in our view, is unnecessarily complicated for low dimensions. The conceptually simplest approach is to perform repeated local minimization from random starting points, thus heuristically (though sufficiently safe) obtaining all global optimal points. Below we describe different possible approaches for local minimization, either applying available optimization algorithms or implementing simple ones ourselves.

In the case that only the optimal value $p^\star$ and not the optimal solution $(\phi^\star, \chi^\star)$ is sought for, a positive maps approach is fruitful. Given an operator $A \in H$ one can define the linear map $L_A$ such that

$$
(\phi \otimes \chi)^\dagger A(\phi \otimes \chi) = \chi^\dagger L_A(\phi \phi^\dagger) \chi.
$$

(147)
Problem (15) is then equivalent to minimizing the smallest eigenvalue of \( L_A(\phi \phi^\dagger) \) as a function of normalized \( \phi \), and hence to the unconstrained minimization of

\[
\tilde{f}_\Omega(\phi) = \min \text{spec} \frac{L_A(\phi \phi^\dagger)}{\phi^\dagger \phi}.
\] (148)

With a real parametrization \( \phi = Jx \) as in equation (117) this function is readily minimized by the Nelder–Mead downhill simplex algorithm, listed e.g. in [62] and implemented e.g. in MATLAB’s “fminsearch” [63] function or Mathematica’s “NMinimize” [64].

In the case that also the optimal point \((\phi^*, \chi^*)\) is sought for several possibilities exist. An approximate solution is easily found by feeding the real problem given by (120) to a SQP-algorithm [42, 65], e.g. the one provided in MATLAB’s “fmincon” function [63]. Another possibility is to apply the infinity norm in (15) and perform box-constrained minimization in each face of the \( \infty \)-ball. Since the Hessian of the function is readily available trust-region algorithms are suitable (also provided in MATLAB’s “fmincon”). If \( A \) is known to be a witness, even the box-constraints on each face of the \( \infty \)-ball can be removed, since in that case the objective function is bounded below. The problem has then been reduced to unconstrained minimization in a series of affine spaces, one for each face of the \( \infty \)-ball. With this latter formulation, we have had success with a quasi-Newton approach [42] performing exact line search, see [37] for details. Further, we have had promising results with a complex conjugate gradient algorithm also performing exact line search [65], though further development is necessary.

B.2 Finding the boundary of a face

Here we describe how to localize the boundary of a quadratic face of \( S_1^\circ \). We assume we have some routine for solving problem (15).

Given a quadratic witness \( \Omega \) situated in the interior of a face defined by \( k \) product vectors, and a perturbation \( \Gamma \), we define a family of functions as follows. Consider problem (15) with \( A(t) = \Omega + t \Gamma \). Given all local minima, sort these in ascending order according to function value. Then the function \( \kappa_0(t) \) is the value of local minimum number \( k + 1 \) if this exists and 0 otherwise. Function \( \kappa_i(t), i = 1, \ldots, k \) is the smallest positive eigenvalue of \( D^2(f_\Omega + t f_\Gamma) \) evaluated at zero number \( i \). Now each \( \kappa_i(t), i = 0, \ldots, k \) is a function with a single simple root in \( t \in [0, \infty) \) which can be easily located using any standard rootfinding technique.

Another possible approach to finding the boundary of the face is as follows. Rather than locating all local minima of problem (15), aim only at locating the global minimum value. This global minimum value as a function of \( \Omega \) will be called the face function. The face function is zero on a face, positive in the interior of \( S_1^\circ \) and negative outside of \( S_1^\circ \). Finding some initial \( \theta > \theta_c \) then allows for one-sided extrapolation towards \( \theta_c \).

If we employ the 2-norm for the constraints in (15) the face function is concave as a function of \( \theta > \theta_0 \). To see this, note that the optimal value of problem (15) is equal to the optimal value of

\[
\tilde{f}(\phi, \chi) = \frac{(\phi \otimes \chi)^\dagger \Omega(\phi \otimes \chi)}{(\phi^\dagger \phi)(\chi^\dagger \chi)}.
\] (149)

Let \( p^*(\Omega) \) denote the optimal value. Since \( p^*(\Omega) \) is defined as a point-wise minimum \( p^*(\Omega) \) is a concave function of \( \Omega \) [41]. Projection of \( \Omega \) on some face is an affine operation, an operation preserving concavity. Accordingly the face function is a concave function once the new local
minimum exists. This fact makes either approach for locating the boundary of a face simpler, since the qualitative form of the function whose root to find is known.

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