Boundary of the set of separable states

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Abstract

Motivated by the separability problem in quantum systems $2 \otimes 4$, $3 \otimes 3$ and $2 \otimes 2 \otimes 2$, we study the maximal (proper) faces of the convex body, $S_1$, of normalized separable states in an arbitrary quantum system with finite-dimensional Hilbert space $H = H_1 \otimes H_2 \otimes \cdots \otimes H_n$. To any subspace $V \subseteq H$ we associate a face $F_V$ of $S_1$ consisting of all states $\rho \in S_1$ whose range is contained in $V$. We prove that $F_V$ is a maximal face if and only if $V$ is a hyperplane. If $V = |\psi\rangle \perp$ where $|\psi\rangle$ is a product vector, we prove that $\text{Dim } F_V = d^2 - 1 - \prod (2d_i - 1)$, where $d_i = \text{Dim } H_i$ and $d = \prod d_i$. We classify the maximal faces of $S_1$ in the cases $2 \otimes 2$ and $2 \otimes 3$. In particular we show that the minimum and the maximum dimension of maximal faces is 6 and 8 for $2 \otimes 2$, and 20 and 24 for $2 \otimes 3$. The boundary, $\partial S_1$, of $S_1$ is the union of all maximal faces. When $d > 6$ we prove that there exist full states on $\partial S_1$, i.e., states $\rho \in \partial S_1$ such that all partial transposes of $\rho$ (including $\rho$ itself) have rank $d$. K.-C. Ha and S.-K. Kye have recently constructed explicit such states in $2 \otimes 4$ and $3 \otimes 3$. In the latter case, they have also constructed a remarkable family of faces, depending on a real parameter $b > 0$, $b \neq 1$. Each face in the family is a 9-dimensional simplex and any interior point of the face is a full state. We construct suitable optimal entanglement witnesses (OEW) for these faces and analyze the three limiting cases $b = 0, 1, \infty$.

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1 Introduction

Let \( \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n \) be the complex Hilbert space of a finite-dimensional \( n \)-partite quantum system. We denote by \( d_i \) the dimension of \( \mathcal{H}_i \), and so \( d := \prod d_i \) is the dimension of \( \mathcal{H} \). To avoid trivial cases, we assume that each \( d_i > 1 \) and \( n > 1 \). Let \( H \) be the space of Hermitian operators \( \rho \) on \( \mathcal{H} \). Note that \( H \) is a real vector space and that \( \text{Dim} H = d^2 \). We denote by \( \mathcal{H}_1 \) the affine hyperplane of \( H \) defined by the equation \( \text{Tr} \rho = 1 \). The mixed quantum states of this quantum system are represented by their density matrices, i.e., operators \( \rho \in H \) which are positive semidefinite \( (\rho \geq 0) \) and have unit trace \((\text{Tr} \rho = 1)\). For convenience, we often work with non-normalized states, i.e., Hermitian operators \( \rho \) such that \( \rho \geq 0 \) and \( \rho \neq 0 \). It will be clear from the context whether we require the states to be normalized.

We denote by \( \mathcal{D}_1 \) and \( \mathcal{D} \) the set of normalized and non-normalized states, respectively. Thus \( \mathcal{D}_1 = \mathcal{D} \cap \mathcal{H}_1 \) is a compact convex subset of \( \mathcal{H}_1 \). We say that an operator \( \rho \in H \) has full rank if it is invertible, and otherwise we say that \( \rho \) has deficient rank. The boundary \( \partial \mathcal{D} \) of \( \mathcal{D} \) (as a subset of \( H \)) consists of the zero operator and all states of deficient rank, i.e.,

\[
\partial \mathcal{D} = \{ \rho \in H : \rho \geq 0, \ \text{rank} \rho < d \}.
\]

We say that a nonzero vector \( |a\rangle \in \mathcal{H} \) is a product vector (or that it is separable) if it is the tensor product \( |a\rangle = |a_1\rangle \otimes \cdots \otimes |a_n\rangle \) of vectors \( |a_i\rangle \in \mathcal{H}_i \). For brevity, we also write it as \( |a\rangle = |a_1, \ldots, a_n\rangle \).

Otherwise we say that \( |a\rangle \) is entangled. A state \( \rho \) is a pure product state if \( \rho = |a\rangle \langle a| \) for some product vector \( |a\rangle \). A state \( \sigma \) is separable if it can be written as a sum of pure product states. We shall denote by \( \mathcal{S}_1 \) and \( \mathcal{S} \) the set of normalized and non-normalized separable states, respectively. Note that both \( \mathcal{D} \cup \{0\} \) and \( \mathcal{S} \cup \{0\} \) are closed convex cones and \( \mathcal{S} \subseteq \mathcal{D} \). We say that a state is entangled if it is not separable. While \( \partial \mathcal{D} \) has a very simple description, the boundary \( \partial \mathcal{S} \) of \( \mathcal{S} \) is well understood only for \( d \leq 6 \). That is, a two-qubit or qubit-qutrit separable state belongs to \( \partial \mathcal{S} \) if and only if it or its partial transpose has deficient rank. The boundary \( \partial \mathcal{S}_1 \) of \( \mathcal{S}_1 \) (as a subset of \( \mathcal{H}_1 \)) and \( \partial \mathcal{S} \) are closely related. Indeed, we have \( \partial \mathcal{S} = \{ tp : \rho \in \partial \mathcal{S}_1, t > 0 \} \). The set \( \mathcal{S}_1 \) is the convex hull of the set of all normalized pure product states. Moreover, the latter set is the set of extreme points of \( \mathcal{S}_1 \).

For any vector subspace \( V \subseteq \mathcal{H} \), we denote by \( P_V \) the set of normalized product vectors contained in \( V \). In particular, \( P_\mathcal{H} \) is the set of all normalized product vectors in \( \mathcal{H} \). Note that \( P_\mathcal{V} = V \cap P_\mathcal{H} \) for any vector subspace \( V \subseteq \mathcal{H} \). Finally, we set \( R_\mathcal{V} := \{ |v\rangle \langle v| : |v\rangle \in P_\mathcal{V} \} \). Thus, \( R_\mathcal{H} \) is the set of all normalized pure product states. The range of a linear operator \( \rho \) will be denoted by \( \mathcal{R}(\rho) \).

The partial transposition operators, \( \Gamma \), form an elementary Abelian group, \( \Theta \), of order \( 2^n \). These operators act on the algebra \( \mathcal{A} \) of all complex linear operators on \( \mathcal{H} \). Their definition depends on the choice of bases in the Hilbert spaces \( \mathcal{H}_i \). We assume that some orthonormal (o.n.) basis \( \{ |j\rangle : 0 \leq j < d_i \} \) of \( \mathcal{H}_i \) is fixed for each \( i \). We use the fact that \( \mathcal{A} \) is the tensor product of the algebras \( \mathcal{A}_i \), \( i = 1, \ldots, n \), of linear operators on \( \mathcal{H}_i \). Thus each \( A \in \mathcal{A} \) can be written as a finite sum of so called local operators (LO), i.e., operators of the form \( \otimes_{i=1}^n A_i \), \( A_i \in \mathcal{A}_i \). The partial transposition operator \( \Gamma_j, j = 1, \ldots, n \), is characterized by the property that it sends \( \otimes_{i=1}^n A_i \rightarrow \otimes_{i=1}^n B_i \), where \( B_i = A_i \) for \( i \neq j \) and \( B_j = A_j^T \) is the transpose of \( A_j \) (computed in our fixed o.n. basis of \( \mathcal{H}_j \)). Obviously, \( \Gamma_i \Gamma_j = \Gamma_j \Gamma_i \) for all \( i \) and \( j \).

We define \( \Theta \) to be the group generated by the \( \Gamma \)'s. For convenience, we set \( \rho^\Gamma = \Gamma(\rho) \). We say that a Hermitian operator \( \rho \in H \) is full if \( \rho^\Gamma \) has full rank for all \( \Gamma \in \Theta \).
We say that a state \( \rho \) on \( \mathcal{H} \) has positive partial transposes (or that it is a PPT state) if \( \rho^\Gamma \geq 0 \) for all \( \Gamma \in \Theta \). We denote by \( \mathcal{P} \) the cone consisting of all non-normalized PPT states, and we set \( \mathcal{P}_1 = \mathcal{P} \cap H_1 \). It follows that \( \mathcal{P}_1 = \cap_{\Gamma \in \Theta} \Gamma(D_1) \). Since each \( \Gamma \in \Theta \) preserves the set \( R_\mathcal{H} \) of normalized pure product states, it also preserves the set \( \mathcal{S}_1 \). In general we have \( \mathcal{S}_1 \subseteq \mathcal{P}_1 \subseteq D_1 \) and the equality \( \mathcal{S}_1 = \mathcal{P}_1 \) holds if and only if \( d \leq 6 \).

We recall some basic notions and terminology concerning compact convex subsets of a Euclidean space. In our case this space will be \( H \) or its affine subspace \( H_1 \). Occasionally we shall apply this terminology to more general convex sets such as \( D, \mathcal{P} \) and \( \mathcal{S} \).

Let \( K \subseteq H_1 \) be any compact convex subset. We denote by \( \text{aff}(K) \) the smallest affine subspace of \( H_1 \) containing \( K \). By definition, the dimension of \( K \) is equal to the dimension of \( \text{aff}(K) \). The relative boundary of \( K \), i.e. as a subset of \( \text{aff}(K) \), will be denoted by \( \partial K \). A face of \( K \) is a convex subset \( F \subseteq K \) such that the conditions \( x, y \in K \) and \( px + (1 - p)y \in F, \) \( 0 < p < 1, \) imply that \( x, y \in F \). The set \( K \) itself is its own face, the unique improper face, all other faces are called proper faces. We say that a proper face \( F \) of \( K \) is exposed if there exists an affine hyperplane \( X \subseteq H_1 \) such that \( X \cap K = F \). Since \( K \) is compact, it is clear that the empty face is exposed. By convention, the improper face is also exposed. A face \( F \) of \( K \) is maximal if there is no face \( F' \) such that \( F \subseteq F' \subseteq K \) and \( F \neq K \). The boundary \( \partial K \) is the union of all maximal faces of \( K \). Given any subset \( X \subseteq K \), there is the smallest (with respect to inclusion) face \( F \) of \( K \) containing \( X \), and we say that the face \( F \) is generated by \( X \).

This paper is motivated by the desire to solve the separability problem for some low-dimensional quantum systems such as \( 2 \otimes 4, 3 \otimes 3, \) and \( 2 \otimes 2 \otimes 2 \). In our previous publication [6, p. 5] we have proposed a method to do that based on the theory of invariants. The recent paper of P. D. Jarvis [22] can be viewed as a first step in that direction. To make further progress, it is necessary to obtain a better understanding of the boundary of the set \( \mathcal{S}_1 \). Our objective is to present some basic facts (old and new) concerning \( \partial \mathcal{S}_1 \) and raise some related challenging problems.

Let \( \Phi_k : H \to \mathbb{R}, \ k = 1, \ldots , d, \) be the polynomial functions defined as follows: \( \Phi_k(\rho) \) is the sum of all \( k \times k \) principal minors of the matrix \( \rho \in H \). Note that \( \Phi_1 = \text{Tr} \). We recall that the affine hyperplane \( H_1 \) is defined by the equation \( \text{Tr}(\rho) = 1 \). The convex body \( D_1 \) can be described as the set of all ponts \( \rho \in H_1 \) satisfying \( d - 1 \) inequalities

\[
\Phi_k(\rho) \geq 0, \quad k = 2, \ldots , d. \tag{2}
\]

We can also define the convex body \( \mathcal{P}_1 \) by a bunch of polynomial inequalities. For each \( \Gamma \in \Theta \) we define the polynomial function \( \Phi_{\Gamma}^k : H \to \mathbb{R} \) by setting \( \Phi_{\Gamma}^k(\rho) = \Phi_k(\rho^\Gamma) \). Then the set \( \mathcal{P}_1 \) can be described as the set of all ponts \( \rho \in H_1 \) satisfying \( 2^n(d - 1) \) inequalities

\[
\Phi_{\Gamma}^k(\rho) \geq 0, \quad \Gamma \in \Theta, \ k = 2, \ldots , d. \tag{3}
\]

The faces of \( D_1 \) are parametrized by vector subspaces \( V \subseteq \mathcal{H} \) [11 section II]. The face \( F_V \) that corresponds to \( V \) consists of all states \( \rho \in D_1 \) such that \( \mathcal{R}(\rho) \subseteq V \). The intersection

\[
F_V := F_V \cap \mathcal{S}_1 = \{ \rho \in \mathcal{S}_1 : \mathcal{R}(\rho) \subseteq V \} \tag{4}
\]

is a face (possibly empty) of \( \mathcal{S}_1 \). We say that the face \( F_V \) is associated to \( V \). As each face of \( D_1 \) is exposed, it follows that each \( F_V \) is an exposed face of \( \mathcal{S}_1 \).

We denote by \( \mathcal{F} \) the set of all faces of \( \mathcal{S}_1 \). Each \( \Gamma \in \Theta \) preserves \( \mathcal{S}_1 \), permutes the faces of \( \mathcal{S}_1 \) and preserve their properties. For any \( F \in \mathcal{F} \), we denote by \( P_F \) the set of product vectors \( |z\rangle \in \mathcal{H} \) such that \( |z\rangle \langle z| \in F \). It is immediate from the definitions that for any subspace \( V \subseteq \mathcal{H} \) we have

\[
P_V = P_{F_V}. \tag{5}
\]
For any $F \in \mathcal{F}$ we set $\mathcal{R}(F) = \sum_{\rho \in F} \mathcal{R}(\rho)$. Thus $\mathcal{R}(F)$ is the smallest subspace of $\mathcal{H}$ which contains $\mathcal{R}(\rho)$ for all $\rho \in F$. It is easy to verify that $\mathcal{R}(F) = \text{span} P_F$ for any $F \in \mathcal{F}$. Note that there always exists $\rho \in F$ such that $\mathcal{R}(\rho) = \mathcal{R}(F)$. Further, we have

$$F \subseteq F_{\mathcal{R}(F)}, \quad \forall F \in \mathcal{F}. \quad (6)$$

Indeed, for $\rho \in F$ we have $\mathcal{R}(\rho) \subseteq \mathcal{R}(F)$ and so $\rho \in F_{\mathcal{R}(F)}$. The inclusion in (6) may be proper (see Example 4).

We say that $F \in \mathcal{F}$ is an induced face if $F = \Gamma(F_V)$ for some subspace $V \subseteq \mathcal{H}$ and some $\Gamma \in \Theta$. Since each face $F_V$ is exposed, the same is true for all induced faces. One defines the induced faces of $S$ similarly. We shall see later (Proposition 3) that when $d > 6$ there exist maximal faces which are not induced. We warn the reader that our definition of induced faces is different from the one adopted in [15] in the bipartite case. It is easy to see that in the bipartite case every induced face $F \in \mathcal{F}$ is also induced according to the definition in that paper. However, the converse is false. A counter-example is provided by the face $F'$ of Proposition 12 when $n = 2$ and $d_1 = d_2 = 2$.

If $F \in \mathcal{F}$ is a proper induced face then $F = \Gamma(F_V)$ for some subspace $V \subseteq \mathcal{H}$ and some $\Gamma \in \Theta$. Thus, $\Gamma(F) = F_V \subseteq \partial \mathcal{D}_1$ and at least one of the functions $\Phi_k^\Gamma, k = 2, \ldots, d$, must vanish on $F$. It follows that the union of all proper induced faces of $S_1$ is equal to $\partial \mathcal{P}_1 \cap S_1$. The points $\rho \in S_1$ satisfy all inequalities (3) but if $d > 6$ they must also satisfy some additional inequalities because $S_1 \subseteq \mathcal{P}_1$. In order to find these additional inequalities we need to construct some non-induced faces $F$ of $S_1$, namely those which are not contained in $\partial \mathcal{P}_1$. Note that if $\rho \in F \in \mathcal{F}$ and $\rho \notin \partial \mathcal{P}_1$ then $\rho$ must be a full state. We shall consider such states in the next section.

Among the three smallest systems with $d > 6$, namely $2 \otimes 4$, $3 \otimes 3$ and $2 \otimes 2 \otimes 2$, proper faces $F \in \mathcal{F}$ not contained in $\partial \mathcal{P}_1$ are known only in $3 \otimes 3$. A remarkable family of such faces, $\Delta_b$, depending on the real parameter $b > 0, b \neq 1$, has been constructed recently in [15], see also Example 4 below. We shall study this family in section 5. In the case $2 \otimes 2 \otimes 2$, no concrete full states on the boundary of $S_1$ are known.

In section 2 we study the separable full states lying on the boundary of $S_1$. In Proposition 2 we show that if $\rho \in S_1$ is a full state, then $\rho \notin \partial S_1$. It follows that such $\rho$ belongs to a proper induced face of $S_1$. In Proposition 3 we show that if a proper face $F$ of $S_1$ contains a full state, then $F$ is not induced. We deduce that $S_1 \cap \partial \mathcal{P}_1$ is the union of all proper induced faces of $S_1$. In the same proposition we also prove that if $d > 6$ then there exist full states lying on $\partial S_1$. In the $2 \otimes 4$ and $3 \otimes 3$ systems infinitely many explicit full states on $\partial S_1$ are known (see [16] and Example 4). In the case $3 \otimes 3$, each face $\Delta_b$ mentioned above is a 9-dimensional simplex and each interior point of $\Delta_b$ is a full state.

In section 3 we consider the special case where $d_1 = \cdots = d_n$ and we use the identifications $\mathcal{H}_1 = \cdots = \mathcal{H}_n$. We denote by $\mathcal{H}_{\text{sym}}$ the subspace of symmetric tensors of $\mathcal{H}$. In Proposition 3 we compute the dimension of the face $F = F_{\mathcal{H}_{\text{sym}}}$ and show that its extreme points are the states $|x, \ldots, x\rangle|x, \ldots, x\rangle$ where $|x\rangle \in \mathcal{H}_1$ and $||x|| = 1$. In Proposition 12 we determine the extreme points of the face $S \cap \Gamma(F)$ as well as the subspace of $H$ spanned by this face. The dimension of this subspace is given by Eq. (21), and $\text{Dim } F$ is just one less.

In section 4 we introduce the $\circ$-action of $\text{GL}$ on $\mathcal{D}_1$ which sends $\rho \in \mathcal{D}_1$ to the normalization of $A \rho A^\dagger$. One of the main results of this section is Proposition 13 where we prove that for every maximal face $F$ of $S_1$ we have $\text{Dim } \mathcal{R}(F) \geq d - 1$. This implies that a maximal face $F$ is induced if and only if $\text{Dim } \mathcal{R}(\Gamma(F)) = d - 1$ for some $\Gamma \in \Theta$. The second main result of this section (Theorem 15) is that the face $F_V$, associated to a subspace $V \subseteq \mathcal{H}$, is maximal if and only if $V$ is a hyperplane. As a corollary we obtain that every hyperplane $V \subseteq \mathcal{H}$ is spanned by product vectors. We compute the dimension of any maximal face $F_V$ where $V = |\alpha\rangle^\perp$ in two cases: first for arbitrary $n$ with $|\alpha\rangle$ a product vector and
second for \( n = 2 \) with \(|\alpha\rangle \) of Schmidt rank two. We also obtain a very simple classification of maximal faces in \( 2 \otimes 2 \) and \( 2 \otimes 3 \) up to the \( \varphi \)-action of \( \text{GL} \).

In section 3 we study the above mentioned family \( \Delta_b, b > 0, b \neq 1 \), of 9-dimensional faces of \( S_1 \) in the \( 3 \otimes 3 \) system. We include the limiting cases \( b = 0, 1, \infty \). We construct entanglement witnesses (EW) \( W_b \) such that \( \Delta_b = \{ \rho \in S_1 : \text{Tr}(\rho W_b) = 0 \} \). When \( b \neq 1 \) then \( W_b \) is in fact an OEW. For \( b \neq 1 \), each interior point of \( \Delta_b \) is a full state and so the face \( \Delta_b \) is not induced. As a by-product of these results we obtain that the set of normalized (i.e., having trace 1) OEW is not closed. This family of states is remarkable as it provides the first examples of non-induced faces of relatively high dimension. No such faces are known in \( 2 \otimes 4 \) and \( 2 \otimes 2 \otimes 2 \) systems. In the \( 2 \otimes 4 \) case, full states on the boundary of \( S_1 \) have been constructed very recently [16].

### 2 Boundary of the set of separable states

#### 2.1 Basic facts

It is well known that \( S_1 \) is a compact convex set and that \( \text{Dim} S_1 = d^2 - 1 \). Let us begin with three observations concerning the boundary of \( S_1 \).

**Observation 1.** \( S_1 \) is not a polytope.

In the bipartite case this been shown in [21]. While the proof given there can be easily extended to the multipartite case, we shall give a slightly different and shorter proof for the general case. Clearly \( S_1 \) has at least one extreme point. As \( S_1 \) is the convex hull of \( R_H \), every extreme point of \( S_1 \) must belong to \( R_H \). Since the local unitary group \( \times_{i=1}^n \text{U}(d_i) \) acts transitively on \( R_H \), each \( \rho \in R_H \) is an extreme point of \( S_1 \). Thus, \( S_1 \) has infinitely many extreme points, and so it is not a polytope.

The set of extreme points of any face \( F \) of \( S_1 \), is just the set \( F \cap R_H \) of all pure product states contained in \( F \). It is not known what is the maximal dimension of the proper faces \( F \) of \( S_1 \).

**Observation 2.** If \( \rho \in S \) has deficient rank then \( \rho \in \partial D \). This follows from the fact that \( \rho \in \partial D \).

In particular, the condition is satisfied if the range of \( \rho \in S \) contains only finitely many product vectors. (We always count the product vectors up to a scalar factor.)

**Observation 3.** The set \( R_V \) is the set of extreme points of \( F_V \). Consequently, \( F_V \) is the convex hull of \( R_V \).

**Proof.** Every extreme point \( \rho \) of \( F_V \) is also an extreme point of \( S_1 \) and so \( \rho = |x\rangle \langle x| \) for some unit product vector \(|x\rangle \). Since \( \rho \in F_V \) we have \(|x\rangle \in V \). Thus \(|x\rangle \in R_V \) and so \( \rho \in R_V \). The converse is obvious. \( \square \)

Very little is known about the set \( F \) of all faces of \( S_1 \). Some proper faces of low dimensions have been explicitly constructed. Most of them are polytopes. Examples of proper faces that are not polytopes can be found in [1]. Such examples exist even in the case of two qubits \((n = d_1 = d_2 = 2)\). Indeed, the face associated to \(|0\rangle \otimes \mathcal{H}_2 \) is \(|0\rangle |0\rangle \otimes B_2 \) where \( B_2 \) is the Bloch ball of the second qubit. By using Observation 3, we can construct a rich family of faces of \( S_1 \) which are polytopes. Under a suitable condition on the \( d_i \), these faces are not simplices.

**Example 1** A generic subspace \( V \subset \mathcal{H} \) of dimension \( d - \sum (d_i - 1) \) contains exactly

\[
N := \frac{(\sum (d_i - 1))!}{\prod ((d_i - 1)!)}
\]

(product vectors). This follows from the fact that \( N \) is the degree of the product of complex projective spaces associated to the \( \mathcal{H}_i, i = 1, \ldots, n \), under the Segre embedding into the projective space associated...
to $\mathcal{H}$ (see [25, p. 412]). Let $|z_i⟩ \in \mathcal{H}_V$, $i = 1, \ldots, N$, be pairwise non-parallel. Then the convex hull $\Pi$ of the states $|z_i⟩⟨z_i|$ is a face of $\mathcal{S}_1$. Each of the states $|z_i⟩⟨z_i|$ is an extreme point of $\Pi$, and $\Pi$ is not a simplex if $N \geq d$. Since the $|z_i⟩$ span $V$ (see [4]), we have $\text{Dim} \Pi \geq d - \sum(d_i - 1)$. This example also shows that the converse of Observation 3 is not valid, e.g., when $N \geq d$. We leave as an open problem the computation of the dimension of $\Pi$. □

Open problem 1. Compute the dimension of the polytope $\Pi$.

Let us remark that if $\rho \in \mathcal{S}$ then in fact $\rho^\Gamma \in \mathcal{S}$ for all $\Gamma \in \Theta$. Since each $\Gamma \in \Theta$ is an invertible linear transformation of $H$ which preserves $\mathcal{S}_1$, it must map faces to faces, preserve their dimensions and other properties of faces such as being exposed, maximal, induced etc. We say that a Hermitian operator $\rho \in H$ is full if $\rho^\Gamma$ has full rank for all $\Gamma \in \Theta$.

Observation 2 can be generalized as follows.

**Proposition 2** If a state $\rho \in \mathcal{S}$ is not full, then $\rho \in \partial \mathcal{S}$.

**Proof.** By the hypothesis, there exists $\Gamma \in \Theta$ such that $\text{rank} \rho^\Gamma < d$. By the above remark $\rho^\Gamma \in \mathcal{S}$ and Observation 2 implies that $\rho^\Gamma \in \partial \mathcal{S}$. As $\Gamma(\partial \mathcal{S}) = \partial \mathcal{S}$, we conclude that $\rho \in \partial \mathcal{S}$. □

### 2.2 Full states on $\partial \mathcal{S}$

We say that an entangled PPT state is a PPTES. Note that the set of all full states $\rho \in H$ is open in $H$, and that all states $\rho$ in the interior of $\mathcal{S}$ are full. If $\rho \in \partial \mathcal{S}$ is a full state then, for sufficiently small $t > 0$, $\rho - tI_d$ is a PPTES. If $d \leq 6$ there are no PPTES and so, in these cases there are no full states on $\partial \mathcal{S}$. In particular, two-qubit proper faces of $\mathcal{S}_1$ do not contain any full state. We shall see in Proposition 3 below that this is not true if $d > 6$. For a concrete example in $3 \otimes 3$ see Example 4 below.

In quantum information, the state $I_d/d$ is regarded as the white noise to the initial normalized PPTES $\rho$. There is a unique $p \in (0, 1)$ such that $\rho(t) := tI_d/d + (1 - t)\rho$ is entangled for $t \in [0, p)$ and $\rho(p) \in \partial \mathcal{S}_1$. The bigger $p$ is, the more robust entanglement of $\rho$ is against the decoherence. For a given $\rho$, it is an important question to analytically compute $p$. It shows how quantum correlation of $\rho$ is removed by decoherence with the environment. However it is usually hard to compute $p$, as there are very few tools to decide whether a PPT state is separable (except in the two-qubit and qubit-qutrit cases [19]). In contrast, starting with a full state $\sigma \in \partial \mathcal{S}_1$, we may choose $\rho = (1 + t)\sigma - tI_d/d$ with small $t > 0$ in which case we have have $p = t/(1 + t)$. It gives us a method of analytically deciding the robustness of a PPTES against the noise. So it is a meaningful problem to construct full states on $\partial \mathcal{S}_1$.

For a long time no explicit full states on $\partial \mathcal{S}_1$ in any quantum systems that we consider were known. As observed above, if $d \leq 6$ there are no such states. Two well known examples of bipartite states with $d_1 = d_2$ are the Werner state [29]

$$I_d - \frac{1}{d_1} \sum_{i,j=0}^{d_1-1} |ij⟩⟨ji|,$$ (8)

and the isotropic state [18]

$$I_d + \sum_{i,j=0}^{d_1-1} |ii⟩⟨jj|.$$ (9)

A family of separable states of full rank on $\partial \mathcal{S}$ in $2 \otimes d_2$ has been constructed in [4, Proposition 5]. It is also known (see [10]) that the multiqubit state

$$I_{2^n} + |\text{GHZ}⟩⟨\text{GHZ}|, \quad (|\text{GHZ}\rangle = |0,\ldots,0⟩ + |1,\ldots,1⟩)$$ (10)
is separable. Although all of these states have full rank and lie on $\partial S$, it turns out that none of them is a full state.

**Proposition 3** If a proper face $F$ of $S_1$ contains a full state, then $F$ is not induced. If $d > 6$ then there exist full states on $\partial S$ (and $\partial S_1$).

**Proof.** Let $\rho \in F$ be a full state. Then $\rho^F$ belongs to the interior of $D_1$ for all $\Gamma \in \Theta$. Consequently, $F$ is not induced. To prove the second assertion, we assume that $d > 6$. Then there exist PPTES and we fix one of them, say $\rho$. The line segment joining $I_d$ to $\rho$ contains a unique point $\sigma \in \partial S$. Since $\rho^F \geq 0$ for all $\Gamma \in \Theta$, it follows that $\sigma^F$ has full rank for all $\Gamma \in \Theta$. Thus $\sigma \in \partial S$ is a full state. □

We point out that the converse of the first assertion is false (see the discussion below Proposition 13).

The first explicit examples of full states on $\partial S_1$ have been constructed recently in [15, p. 18], see the example below. (Our terminology has not been used in that paper.) We shall analyze this family in more details in section 5.

**Example 4** Let us consider the bipartite system $3 \otimes 3$. In the paper [15] the authors have constructed 10 normalized real product vectors $|z_i\rangle, i = 1, \ldots, 10$, depending on one real parameter $b > 0$, $b \neq 1$. It is easy to verify that any 9 of them are linearly independent. They have shown that the convex hull, $\Delta_b$, of the 10 states $|z_i\rangle|z_i\rangle$ is a 9-dimensional simplex and that $\Delta_b \in F$. Thus $R(\Delta_b) = H$ and $\Delta_b \subset F_H = S_1$. Since all vectors $|z_i\rangle$ are real, it follows that $\rho^{F_1} = \rho$. Hence, each interior point $\rho$ of $\Delta_b$ is a full state. By Proposition 3 the face $\Delta_b$ (as well as any proper face containing it) is not induced. □

The full states on $\partial S_1$ in the above example have unique decomposition as the convex sum of pure product states. This is not surprising because separable states with a unique decomposition evidently belong to $\partial S_1$. However the converse is not true. For example, for $n = 2$ any state $|0\rangle|0\rangle \otimes \sigma$, where $\sigma$ is a mixed state, has infinitely many decompositions as the convex sum of pure product states.

In contrast to Example 4 we claim that in the $2 \otimes 4$ system there is no full state $\rho \in \partial S$ such that $\rho^{F_1} = \rho$. Suppose there is such a state $\rho$. Then $\sigma := \rho - tI_8$ is a PPTES for small $t > 0$. As $\sigma^{F_1} = \sigma$, this contradicts [23, Theorem 2]. However, we do not know whether in this system there is a full state $\rho \in \partial S$ such that $\rho^{F_2} = \rho$.

**Open problem 2.** Construct a concrete example of a full state on $\partial S$ in the $2 \otimes 2 \otimes 2$ system.

The following lemma shows that suitable tensor products are full separable states lying on $\partial S$. We define the tensor product of two $n$-partite states, $\rho_{A_1,\ldots,A_n}$ acting on $H_A$ and $\sigma_{B_1,\ldots,B_n}$ acting on $H_B$, as a new $n$-partite state $(\rho \otimes \sigma)_{C_1,\ldots,C_n}$ acting on $H_C$ where each system $C_i$ is obtained by combining $A_i$ and $B_i$ into one system. We shall use subscripts $A, B, C$ to distinguish these three $n$-partite systems. E.g., $I_C$ is the identity operator on $H_C$, and $S_C$ is the cone of non-normalized separable states in $H_C$, etc.

**Lemma 5** Let $\rho \in S_A$ and $\sigma \in S_B$ be full states normalized so that $\text{Tr}(\rho - I_A) = \text{Tr}(\sigma - I_B) = 0$. Then $\alpha := \rho \otimes \sigma$ is a full separable state. Moreover, $\alpha \in \partial S_C$ if and only if $\rho \in \partial S_A$ or $\sigma \in \partial S_B$.

**Proof.** The first assertion is obvious. To prove the second assertion, assume that $\alpha$ is an interior point of $S_C$. Then $\alpha - tI_C \in S_C$ for small $t > 0$. By tracing out the systems $B_1, \ldots, B_n$, we see that $\rho - tI_A \in S_A$ for small $t > 0$. Thus, $\rho$ must belong to the interior of $S_A$. Similarly, $\sigma$ belongs to the interior of $S_B$. Conversely, assume that $\rho$ and $\sigma$ are interior points of $S_A$ and $S_B$, respectively. Then there is a $t > 0$ such that $\rho - tI_A \in S_A$ and $\sigma - tI_B \in S_B$. It follows easily that $\alpha - t^2I_C \in S_C$. Hence, $\alpha$ is an interior point of $S_C$. □
Let $\rho \in \partial S_A$ be any full two-qutrit state mentioned in Example\textsuperscript{4}. It follows from Lemma\textsuperscript{5} that the bipartite separable state $\rho \otimes I_{s_1 s_2}$ is a full state on $\partial S$ on the space $(C^3 \otimes C^{s_1}) \otimes (C^3 \otimes C^{s_2})$ for any positive integers $s_1, s_2$.

So far we have discussed the full separable states of bipartite systems. Here we construct some full states on $\partial S$ in multipartite systems. Let $\rho$ and $\sigma$ be $l$ and $m$-partite separable states, respectively. We regard $\beta = \rho \otimes \sigma$ as a $(l + m)$-partite separable state. If $\rho$ or $\sigma$ is a full state on $\partial S$, then so is $\beta$. This assertion follows from the fact that a state $\beta - tI_d$ is entangled for $t > 0$. Let $\rho$ be the two-qutrit full state on $\partial S$ constructed in Example\textsuperscript{4} so $l = 2$. By choosing a separable state $\sigma$, with $m$ arbitrary, we obtain a full state $\beta$ on $\partial S$ in a multipartite system.

To conclude this section, we present the following observation concerning the full states on $\partial S$.

**Lemma 6** Suppose $\rho \in \partial S$ is a full state. Then there exists $|\psi\rangle \in H$ such that $p\rho + |\psi\rangle \langle \psi|$ is entangled for all $p \geq 0$.

**Proof.** Since $\rho$ has full rank, there exists $t > 0$ such that $\rho - tI_d > 0$. Thus, we have $\rho - tI_d = \sum_i |\psi_i\rangle \langle \psi_i|$ where the sum is finite. Assume that for each $i$ there is a $p_i \geq 0$ such that $p_i := p_i \rho + |\psi_i\rangle \langle \psi_i| \in S$. The identity $\rho - stI_d = (1-s(1+\sum p_i))\rho + s \sum_i p_i$ is valid for all real $s$. Consequently, for small $s > 0$ we have $\rho - stI_d > 0$ which contradicts the fact that $\rho \in \partial S$. Hence, for at least one index $i$ the state $p\rho + |\psi_i\rangle \langle \psi_i|$ must be entangled for all $p \geq 0$.

The lemma implies that some entangled state $|\psi\rangle$ may be “eternally” robust to some separable state $\rho$, which is regarded as noise in quantum information. When $\rho$ is large, the entangled state $p\rho + |\psi\rangle \langle \psi|$ will become a PPTES.

Let us say that a point $\sigma \in \partial S_1$ is a smooth point of $\partial S_1$ if the intersection of $\partial S_1$ with a small ball $B_\varepsilon := \{\rho \in H : ||\rho - \sigma|| < \varepsilon\}$ is a smooth manifold. In connection with the Example\textsuperscript{4} we ask whether the full states belonging to the polytope $\Pi$ are smooth.

### 3 Some faces of $S_1$ when $d_1 = \cdots = d_n$

The following lemma and its corollary will be used in several subsequent proofs.

**Lemma 7** Let $z_1, \ldots, z_m$ be independent complex variables and $n$ a positive integer. Then the monomials $z_1^{j_1}(z_1^*)^{k_1} \cdots z_m^{j_m}(z_m^*)^{k_m}$, where $j_1, k_1, \ldots, j_m, k_m$ are nonnegative integers, are linearly independent over complex numbers. More precisely, if $P := P(x_1, y_1, \ldots, x_m, y_m)$ is a polynomial with complex coefficients in $2m$ independent commuting variables $x_1, y_1, \ldots, x_m, y_m$ and $P(z_1, z_1^*, \ldots, z_m, z_m^*)$ is identically zero, then $P = 0$, i.e., all coefficients of $P$ are zero.

**Proof.** We use induction on $m$. The assertion is obviously valid when $m = 1$, i.e., $z_1$ and $z_1^*$ are algebraically independent over $C$. Assume that $m > 1$. We have $P = \sum_{j,k} x_j^k y_m^k P_{j,k}(x_1, y_1, \ldots, x_{m-1}, y_{m-1})$, where $P_{j,k}$ are polynomials in the $2(m-1)$ variables. By the hypothesis of the lemma we have the identity

$$\sum_{j,k} z_m^j(z_m^*)^k P_{j,k}(z_1, z_1^*, \ldots, z_{m-1}, z_{m-1}^*) = 0.$$ 

Since $z_1$ and $z_1^*$ are algebraically independent over $C$, we deduce that each coefficient $P_{j,k}(z_1, z_1^*, \ldots, z_{m-1}, z_{m-1}^*)$ is identically zero. By the induction hypothesis, we conclude that each polynomial $P_{j,k}(x_1, y_1, \ldots, x_{m-1}, y_{m-1})$ is zero. Consequently, $P = 0$.

The following corollary is an easy consequence of the lemma.
Corollary 8 Let \( \mu_1, \mu_2, \ldots, \mu_s \) be distinct monomials in the complex variables \( z_1, \ldots, z_m \) and their conjugates \( \bar{z}_1, \ldots, \bar{z}_m \). Assume that this list of monomials contains exactly a real-valued monomials, exactly \( b \) pairs \( \{ \mu, \mu^* \} \), (\( \mu^* \neq \mu \)), of complex-conjugate monomials, and \( c \) additional complex-valued monomials. (Thus \( s = a + 2b + c \).) Let \( V \) be a complex vector space and \( v_1, \ldots, v_s \) linearly independent vectors of \( V \). If \( L \) is the real span of the set of vectors \( \{ \sum_{k=1}^{s} \mu_k v_k : z_1, \ldots, z_m \in \mathbb{C} \} \), then \( \text{Dim } L = a + 2(b + c) \).

We can write any linear operator \( L \) on \( \mathcal{H} \) as

\[
L = \sum L^{j_1, \ldots, j_n}_{k_1, \ldots, k_n} |j_1, \ldots, j_n\rangle \langle k_1, \ldots, k_n|,
\]

where the summation is over all \( j_i, k_i \in \{0, 1, \ldots, d_i - 1\}, i = 1, \ldots, n \), and the components (we refer to them also as “matrix coefficients”) are given by \( L^{j_1, \ldots, j_n}_{k_1, \ldots, k_n} = \langle j_1, \ldots, j_n | L | k_1, \ldots, k_n \rangle \).

In this section we assume that \( \mathcal{H}_1 = \cdots = \mathcal{H}_n \) and so \( \mathcal{H} = \otimes^n \mathcal{H}_1 \). We denote by \( \mathcal{H}_{\text{sym}} \) the subspace of \( \mathcal{H} \) consisting of symmetric tensors. We say that \( L \) is range-symmetric if \( \mathcal{R}(L) \subseteq \mathcal{H}_{\text{sym}} \). We warn the reader that the matrix of a range-symmetric operator is not necessarily symmetric. One can recognize whether \( L \) is range-symmetric by examining its matrix coefficients. This is the case if and only if the \( L_{k_1, \ldots, k_n}^{j_1, \ldots, j_n} \) are invariant under the permutations of the superscripts \( j_1, \ldots, j_n \). If \( L \) is Hermitian, this implies that the \( L_{k_1, \ldots, k_n}^{j_1, \ldots, j_n} \) are also invariant under the permutations of the subscripts \( k_1, \ldots, k_n \). We shall denote by \( H_s \) the subspace of \( \mathcal{H} \) consisting of all range-symmetric operators,

\[
H_s = \{ \rho \in \mathcal{H} : \mathcal{R}(\rho) \subseteq \mathcal{H}_{\text{sym}} \}. \tag{12}
\]

Since the space \( \mathcal{H}_{\text{sym}} \) has (complex) dimension \( \binom{n+d_1-1}{n} \), we have

\[
\text{Dim } H_s = \binom{n+d_1-1}{n}^2. \tag{13}
\]

3.1 The face \( F_{\mathcal{H}_{\text{sym}}} \)

We consider here the induced face \( F_{\mathcal{H}_{\text{sym}}} \) of \( S_1 \). In view of (12) we have

\[
F_{\mathcal{H}_{\text{sym}}} = H_s \cap S_1. \tag{14}
\]

We shall describe the set of extreme points of this face and compute its dimension.

For any nonzero \( W \in \mathcal{H} \) we denote by \( X_W \) the hyperplane of \( \mathcal{H} \) defined by the equation \( \text{Tr}(W \rho) = 0 \), and we set \( F_W = X_W \cap S_1 \). If \( \text{Tr}(W \rho) \geq 0 \) for all \( \rho \in S_1 \), then \( F_W \) is an exposed proper face of \( S_1 \) (possibly empty).

Proposition 9 Let \( W_s = I_d - P_s \), where \( P_s \in H_s \) is the projector onto \( \mathcal{H}_{\text{sym}} \), and let \( F \) be the convex hull of the set of operators \( |x, \ldots, x\rangle \langle x, \ldots, x| \in \mathcal{H} \) with \( |x\rangle \in \mathcal{H}_1 \) and \( ||x|| = 1 \).

(i) For any product vector \( |x_1, \ldots, x_n\rangle \in \mathcal{H} \), we have \( \langle x_1, \ldots, x_n | W_s | x_1, \ldots, x_n \rangle \geq 0 \) and the equality holds if and only if all \( |x_i\rangle \) are parallel to each other. Moreover, \( F = F_{\mathcal{H}_{\text{sym}}} \).

(ii) The subspace \( H_s \) is spanned by \( F \) and

\[
\text{Dim } F = \binom{n+d_1-1}{n}^2 - 1. \tag{15}
\]
Proof. (i) We may assume that $|x_i| = 1$ for each $i$. Then $\langle x_1, \ldots, x_n | W_s | x_1, \ldots, x_n \rangle = 1 - \|P_s | x_1, \ldots, x_n \| ^2 \geq 0$ and the equality holds if and only if $|x_1, \ldots, x_n \rangle \in \mathcal{H}_{\text{sym}}$, i.e., if and only if the $|x_i\rangle$ are parallel to each other. It follows that $F = X_{W_s} \cap \mathcal{S}_1$. As $H_s \subseteq X_{W_s}$, we have $F_{\mathcal{H}_{\text{sym}}} \subseteq F$. The opposite inclusion is immediate from the definition of $F$. Hence, we have $F = F_{\mathcal{H}_{\text{sym}}}$. 

(ii) To prove the first assertion of (ii), note that $\langle x_1, \ldots, x | L | x_1, \ldots, x \rangle = 0$ for all $|x\rangle \in \mathcal{H}_1$. Assume that the assertion is false. Then there exists a nonzero $L \in H_s$ such that $\langle x_1, \ldots, x | L | x_1, \ldots, x \rangle = 0$ for all $|x\rangle \in \mathcal{H}_1$. By using the expansion $\langle x_1, \ldots, x \rangle = \sum_{j=0}^{d_1-1} | x_j \rangle | j \rangle$, we obtain that 

$$\sum L_{j_1, \ldots, j_n}^{k_1, \ldots, k_n} \xi_{j_1}^* \cdots \xi_{j_n}^* \xi_{k_1} \cdots \xi_{k_n} = 0,$$

where the summation is over all pairs of repeated indexes, each index running through the integers $0, 1, \ldots, d_1 - 1$. Since $L$ is range-symmetric and Hermitian, the components $L_{j_1, \ldots, j_n}^{k_1, \ldots, k_n}$ are invariant under the permutation of the subscripts or superscripts. By collecting the like terms in (16), we obtain the identity 

$$\sum_{0 \leq j_1 \leq \cdots \leq j_n < d_1} \mu_{j_1, \ldots, j_n}^{k_1, \ldots, k_n} L_{j_1, \ldots, j_n}^{k_1, \ldots, k_n} \xi_{j_1}^* \cdots \xi_{j_n}^* \xi_{k_1} \cdots \xi_{k_n} = 0,$$

where $\mu_{j_1, \ldots, j_n}^{k_1, \ldots, k_n}$ are some positive integers. By Lemma 7 all components $L_{j_1, \ldots, j_n}^{k_1, \ldots, k_n}$ must vanish. Thus $L = 0$ and we have a contradiction.

The second assertion follows from (13) by taking into account that $F \subseteq H_1$. 

For any $\Gamma \in \Theta$ the image $\Gamma(H_s \cap \mathcal{S}_1) = \Gamma(H_s) \cap \mathcal{S}_1$ is also a face of $\mathcal{S}_1$ having the same dimension as $H_s \cap \mathcal{S}_1$. Consequently, the following corollary is valid.

Corollary 10 Let $S$ be any subset of $\{1, \ldots, n\}$ and $\Gamma_S = \prod_{i \in S} \Gamma_i$. For any $|x\rangle \in \mathcal{H}_1$ we set $|x_S\rangle := |x_1, \ldots, x_n\rangle$ where $|x_i\rangle = |x_i^*\rangle$ for $i \in S$ and $|x_i\rangle = |x_i\rangle$ otherwise. Then the face $\Gamma_S(H_s) \cap \mathcal{S}_1$ is the convex hull of all $|x_S\rangle |x_S\rangle$ where $|x\rangle$ runs over all unit vectors in $\mathcal{H}_1$.

Let $H_s^{\text{re}}$ denote the subspace of $H$ consisting of the operators $L$ such that all matrix coefficients of $L$ are real. We remark that the dimension of the subspace $H_s^{\text{re}} := H_s^{\text{re}} \cap H_s$ is given by 

$$\text{Dim } H_s^{\text{re}} = \frac{1}{2} \left( \binom{n + d_1 - 1}{n} \right) \left[ \binom{n + d_1 - 1}{n} + 1 \right].$$

To prove this formula, let us denote by $\mathcal{H}_s^{\text{re}}$ the real Hilbert space consisting of all $|x\rangle = \sum_{j=0}^{d_1-1} | x_j \rangle | j \rangle$ with all $|x_j\rangle$ real, and let $\mathcal{H}_s^{\text{re}} = \otimes_n^\mathbb{R} \mathcal{H}_s^{\text{re}}$ be the real subspace of $\mathcal{H}$ consisting of the tensors having all components real. Then the space $H_s^{\text{re}}$ can be identified with the space of symmetric and range-symmetric operators on $H_s^{\text{re}}$. Now the formula (18) follows from the fact that the space of the symmetric tensors in $\mathcal{H}_s^{\text{re}}$ has dimension $\binom{n + d_1 - 1}{n}$.

Let $H^{\Theta}$ denote the subspace of $H$ consisting of all operators $L$ fixed under $\Theta$, i.e.,

$$H^{\Theta} = \{ L \in H : L^\Gamma = L, \ \forall \Gamma \in \Theta \}. \quad (19)$$

Its dimension was computed in general (for arbitrary $d_1, \ldots, d_n$) in [6] where it was also observed that $H^{\Theta} \subseteq H_s^{\text{re}}$. Finally, we set $H_s^{\Theta} = H^{\Theta} \cap H_s$. 

Let $\Lambda_m$ be the set of all weakly increasing sequences $l = (l_1, l_2, \ldots, l_m)$ of integers $l_i \in \{0, 1, \ldots, d_1 - 1\}$. We shall write $(j_1, \ldots, j_m) \rightarrow (l_1, \ldots, l_m)$ if $(l_1, \ldots, l_m) \in \Lambda_m$ and there is a permutation $\sigma$ of $\{1, \ldots, m\}$ such that $j_{\sigma i} = l_i$ for all $i$.
For each \( l \in \Lambda_{2n} \), let
\[
\rho[l] := \sum_{(j_1, \ldots, j_n, k_1, \ldots, k_n) \neq l} |j_1, \ldots, j_n; k_1, \ldots, k_n|.
\] (20)

It is easy to verify that \( \rho[l] \in H^\Theta_s \) for all \( l \in \Lambda_{2n} \). We claim that the set \( \{ \rho[l] : l \in \Lambda_{2n} \} \) is a basis of \( H^\Theta_s \). It is obvious that this is an orthogonal set of vectors in \( H^\Theta_s \). Let \( L \in H^\Theta_s \) be arbitrary. We can write it as in (11). Since \( H^\Theta_s \subseteq H^{re} \), all components \( L_{k_1, \ldots, k_n}^{j_1, \ldots, j_n} \) are real. Moreover, we know that if \( (j_1, \ldots, j_n, k_1, \ldots, k_n) \to l \), then \( L_{k_1, \ldots, k_n}^{j_1, \ldots, j_n} = L_{k_1+1, \ldots, k_n}^{j_1, \ldots, j_n} \). This means that \( L \) is a real linear combination of the set \( \{ \rho[l] : l \in \Lambda_{2n} \} \) and our claim is proved. Consequently,
\[
\text{Dim } H^\Theta_s = \left( \frac{2n + d_1 - 1}{2n} \right).
\] (21)

3.2 The intersection of all \( \Gamma(H_s) \cap S_1, \Gamma \in \Theta \)

Since \( H_s \cap S_1 \) is a face of \( S_1 \), the same is true for its image \( \Gamma(H_s) \cap S_1 \) under \( \Gamma \in \Theta \). Our objective here is to determine the intersection of all these faces. For that purpose we need the following proposition.

**Proposition 11** We have \( H^\Theta_s = \cap_{\Gamma \in \Theta} \Gamma(H_s) = H_s \cap \Gamma_1(H_s) \).

**Proof.** Obviously, we have \( H^\Theta_s \subseteq \cap_{\Gamma \in \Theta} \Gamma(H_s) \subseteq H_s \cap \Gamma_1(H_s) \). Hence, it suffices to show that \( H_s \cap \Gamma_1(H_s) \subseteq H^\Theta_s \). Let \( L \in H_s \cap \Gamma_1(H_s) \) be arbitrary and write it as in (11). We have to show that \( L \in H^\Theta_s \), i.e., that the components \( L_{j_1, \ldots, j_n}^{k_1, \ldots, k_n} \) remain unchanged when we permute arbitrarily the \( 2n \) indexes \( j_1, \ldots, j_n, k_1, \ldots, k_n \). Since \( L \in H_s \), we know that these components do not change when we permute the superscripts and subscripts separately. As
\[
L_{j_1, j_2, \ldots, j_n}^{k_1, k_2, \ldots, k_n} = \sum L_{j_1, j_2, \ldots, j_n}^{k_1, k_2, \ldots, k_n} |j_1, j_2, \ldots, j_n; k_1, k_2, \ldots, k_n| \in H_s, \tag{22}
\]
the components \( L_{j_1, j_2, \ldots, j_n}^{k_1, k_2, \ldots, k_n} \) are unchanged when we permute the indexes \( j_1, j_2, \ldots, j_n \). Equivalently, the components \( L_{k_1, k_2, \ldots, k_n}^{j_1, j_2, \ldots, j_n} \) are unchanged when we permute the indexes \( k_1, k_2, j_3, \ldots, j_n \).

For convenience, let us label the superscripts \( j_1, \ldots, j_n \) and the subscripts \( k_1, \ldots, k_n \) of \( L_{k_1, k_2, \ldots, k_n}^{j_1, j_2, \ldots, j_n} \) with integers \( 1, \ldots, n \) and \( n + 1, \ldots, 2n \), respectively. The symmetric group \( S_{2n} \) permutes the set \( \Omega := \{1, 2, \ldots, 2n\} \). We single out the three subgroups of \( S_{2n} \), each isomorphic to \( S_n \): the first one permutes only the integers \( 1, \ldots, n \), the second one permutes only the integers \( n + 1, \ldots, 2n \), and the third permutes only the integers \( 2, 3, \ldots, n, n + 1 \). We have shown above that the components \( L_{k_1, k_2, \ldots, k_n}^{j_1, j_2, \ldots, j_n} \) are not changed when we permute the indexes by using a permutation belonging to one of these three copies of \( S_n \). Now our assertion follows from the fact that these three copies of \( S_n \) generate the whole group \( S_{2n} \).

To prove this fact, let us denote by \( G \) the subgroup of \( S_{2n} \) generated by our three copies of \( S_n \). It is obvious that \( G \) acts transitively on the set \( \Omega \). It is also obvious that \( G \) is primitive, i.e., there is no proper subset \( \Delta \) of \( \Omega \) of cardinality at least 2 such that for each \( g \in G \) either \( g(\Delta) = \Delta \) or \( g(\Delta) \cap \Delta = \emptyset \). Since \( G \) contains a transposition, we must have \( G = S_{2n} \) (see e.g., [20, Chap. II, Satz 4.5]). \( \square \)

As an example, we mention that in the case \( n = 2 \), \( d_1 = d_2 = 3 \), the spaces \( H, H^{re}, H_s, H^\Theta \) have dimensions 81, 45, 36, 36 and 15, respectively.

**Proposition 12** Let \( F \) be the face \( F_{H^{sym}} \) of \( S_1 \) and let \( F' := \cap_{\Gamma \in \Theta} \Gamma(F) \).

(i) The operators \( |x, \ldots, x; x, \ldots, x| \in H \) with \( |x| \in H_1^{re} \) span the space \( H^\Theta_s \).

(ii) The face \( F' \) is the convex hull of all \( |x, \ldots, x; x, \ldots, x| \in H \) with \( |x| \in H_1^{re} \) and \( \|x\| = 1 \).

(iii) \( F' \) is neither induced nor a polytope.
Proof. (i) Note first that \(|x, \ldots, x\rangle \langle x, \ldots, x| \in H_s^\Theta\) for all \(|x\rangle \in \mathcal{H}^e_1\). Assume that the assertion is false. Then there exists a nonzero \(L \in H_s^\Theta\) such that \(\langle x, \ldots, x|L|x, \ldots, x\rangle = 0\) for all \(|x\rangle \in \mathcal{H}^e_1\). By using the expansion \(|x\rangle = \sum_{j=0}^{d_1-1} \xi_j|j\rangle\), we obtain that
\[
\sum_{k_1, \ldots, k_n} L_{k_1, \ldots, k_n} \xi_{j_1} \cdots \xi_{j_n} \xi_{k_1} \cdots \xi_{k_n} = 0,
\]
where the summation is over all pairs of repeated indexes, each index running through the integers 0, 1, \ldots, \(d_1-1\). Recall that the components \(L_{k_1, \ldots, k_n}\) are symmetric in the subscripts and the superscripts. Moreover, since \(L \in H^\Theta\), these components are not changed if we switch one of the subscripts with one of the superscripts. Hence, by collecting the like terms in (16), we obtain an identity
\[
\sum_{1 \leq m_1 \leq \cdots \leq m_{2n} \leq 2n} \mu'_{m_1, \ldots, m_{2n}} L_{m_1, \ldots, m_{2n}}^{m_1, \ldots, m_{n}} \xi_{m_1} \cdots \xi_{m_{2n}} = 0,
\]
where \(\mu'_{m_1, \ldots, m_{2n}}\) are some positive integers. Since the monomials \(\xi_{m_1} \cdots \xi_{m_{2n}}, 1 \leq m_1 \leq \cdots \leq m_{2n} \leq 2n\), are linearly independent, all components \(L_{k_1, \ldots, k_n}\) must vanish. Thus \(L = 0\) and we have a contradiction.

(ii) By Proposition \([\[\]\]\) we have
\[
F' = \cap_{\Gamma \in \Theta} (\Gamma(H_s) \cap S_1) = (\cap_{\Gamma \in \Theta} \Gamma(H_s)) \cap S_1 = H_s^\Theta \cap S_1.
\]
Note that \(H_s^\Theta \cap S_1\) is a face of \(F\). Hence, every extreme point \(\rho\) of \(H_s^\Theta \cap S_1\) is also an extreme point of \(F\). By Proposition \([\[\]\]\) we have \(\rho = \langle x, \ldots, x|\langle x, \ldots, x|\) for some unit vector \(|x\rangle \in \mathcal{H}_1\). Since \(\rho \in H^e_1\), it follows that \(\rho^{F_1} = \rho\) and so \(|x^{*}x^*| = |x\rangle \langle x|\). Thus, up to a phase factor, \(|x\rangle \in \mathcal{H}^e_1\) and the assertion is proved.

(iii) Assume that \(F'\) is induced, i.e., \(F' = \Gamma(F_V)\) for some \(\Gamma \in \Theta\) and some subspace \(V \subseteq \mathcal{H}\). By (ii) \(P_{F'}\) consists of real product vectors (up to a phase factor). It follows that \(F' = F_V\). By \([\[\]\]\) we have \(P_{F'} = P_{F_V} = P_V\). Hence \(\mathcal{H}_{\text{sym}} = \mathcal{R}(F') = \text{span} \mathcal{P}_V \subseteq V\). Consequently, \(P_{\mathcal{H}_{\text{sym}}} \subseteq P_V = P_{F'}\). If \(|x\rangle \in \mathcal{H}_1\) is a unit vector which is not real (up to a phase factor), then \(|x\rangle \langle x, x| \in P_{\mathcal{H}_{\text{sym}}} \setminus P_{F'}\) and we have a contradiction. Thus, \(F'\) is not induced. As the set of extreme points of \(F'\) is infinite, \(F'\) is not a polytope.

We remark that the face \(F'\) is exposed because by its definition it is the intersection of exposed faces.

\section{Induced maximal faces of \(S_1\)}

The problem of describing the proper faces of \(S_1\) can be split into two steps: first describe all maximal faces and second describe the proper faces of the maximal faces. To simplify this problem further, we can use the group \(GL := \times_{i=1}^n \text{GL}(d_i)\) which acts on \(\mathcal{H}\) as the group of invertible local operators (ILO). The linear action of \(A \in GL\) sends \(|x\rangle \in \mathcal{H}\) to \(A|x\rangle\). By the induced action on \(H\), \(A\) sends \(\rho \in H\) to \(A\rho A^\dagger\). The former action does not preserve the norm of vectors, and the latter does not preserve the trace of the Hermitian operators. Hence, we are forced to use the actions where \(A\) sends \(|x\rangle \to A|x\rangle := A|x\rangle/\|Ax\|\) and sends \(\rho \to A \circ \rho := (A\rho A^\dagger)/\text{Tr}(A\rho A^\dagger)\). The \(\circ\)-action is well defined on the set \(D_1\). One can easily verify that it maps \(S_1\) onto itself, and preserves the convexity property. Moreover, it permutes the faces of \(S_1\), preserves their dimensions, as well as the properties of being maximal or exposed. Instead of classifying the faces of \(S_1\) up to the action of the local unitary group, we shall consider the easier problem of classifying the faces up to the above \(\circ\)-action of GL. We say that two faces \(F, F' \in \mathcal{F}\) are \(\text{GL-equivalent}\) if \(F' = A \circ F\) for some \(A \in \text{GL}\).
For any subspace \( V \subseteq \mathcal{H} \) we have
\[
A \diamond R_V = \{ \frac{A|v⟩⟨v|A^†}{∥Av∥^2} : |v⟩ \in P_V \} = R_{AV},
\] (25)
and consequently
\[
A \diamond F_V = F_{AV}, \quad A \in \text{GL}.
\] (26)

It follows that the \( \diamond \)-action maps induced faces to induced faces.

If a subspace \( V \subseteq \mathcal{H} \) has dimension \(< d - 1 \), then it is easy to see that the face \( F_V \) is proper but not maximal. Indeed, there exist \( |v⟩ \in P_{\mathcal{H}} \setminus V \) and so if \( V' = V + C|v⟩ \) then \( F_V \subset F_{V'} \subset S_1 \).

**Proposition 13** If \( F \) is a maximal face of \( S_1 \), then \( \dim R(F) \geq d - 1 \). Consequently, a maximal face \( F \in \mathcal{F} \) is induced if and only if \( \dim R(\Gamma(F)) = d - 1 \) for some \( \Gamma \in \Theta \).

**Proof.** Let \( F \in \mathcal{F} \) be such that \( \dim R(F) \leq d - 1 \). Choose a hyperplane \( V \) of \( \mathcal{H} \) such that \( R(F) \subset V \). Then \( F \subseteq F_{R(F)} \subset F_V \subset S_1 \) and so \( F \) is not maximal. The first assertion follows. Next we prove the second assertion. The necessity of the condition follows from the definition of induced faces and the first assertion. To prove the sufficiency, assume that \( F \) is a maximal face and that \( \dim R(\Gamma(F)) = d - 1 \) for some \( \Gamma \in \Theta \). We have to show that the face \( F \) is induced. Without any loss of generality we may assume that \( \Gamma \) is the identity, i.e., that \( \dim R(F) = d - 1 \). As \( F \) is maximal, (6) implies that \( F = F_{R(F)} \) and so \( F \) is an induced face of \( S_1 \).

To illustrate Proposition 13 we mention three examples. The face \( \Delta_b \) in Example 4 is not maximal, see [13, p. 147]. For any face \( F \) containing \( \Delta_b \) we have \( \Gamma(\mathcal{H}) = \Delta_b \) for all \( \Gamma \in \Theta \) which implies that \( R(\Gamma(F)) = \mathcal{H} \). Let \( |z_i⟩, i = 1, \ldots, 10 \) be as in that example. For \( k \in \{1, \ldots, 10\} \) let \( F_k \) denote the maximal face of \( \Delta_b \) not containing the vertex \( |z_k⟩⟨z_k| \). Since any nine vectors \( |z_i⟩ \) span \( \mathcal{H} \), we have \( R(F_k) = \mathcal{H} \) for each \( k \). If \( F' \) is a maximal face of \( F_k \) then \( R(F') \subset \mathcal{H} \) is a hyperplane, but \( F' \) is not a maximal face of \( S_1 \).

The next two examples refer to the maximal faces of two qubits which we shall construct in Proposition 20 below. For \( F = F_{V_1} \) we have \( \dim R(\Gamma(F)) = d - 1 \) for all \( \Gamma \in \Theta \). For \( F = F_{V_2} \) we have \( \dim R(F) = d - 1 \) while \( \dim R(\Gamma_1(F)) = d \).

There is a proper non-maximal face \( F \) of \( S_1 \) such that \( R(F) = \mathcal{H} \) and \( F \) is not a polytope. For example, we can take \( F \) to be the convex hull of the product states \( |x, x⟩′⟨x, x| \) with \( ||x|| = 1 \) and \( d_1 > 2 \). Evidently \( F \in \mathcal{F} \). One can verify that \( R(F) = \mathcal{H} \) and \( \dim R(Γ(F)) < d - 1 \) for all \( Γ \in \Theta \) and \( n = 2 \). It follows from Proposition 13 that \( F \) is not maximal.

Let us also comment on the recent paper [13] where the authors have constructed in \( 2 \otimes 4 \) a face \( F \in \mathcal{F} \) which is the convex hull of ten points \( |z_1⟩⟨z_1|, |z(α_i)⟩⟨z(α_i)|, i = 2, \ldots, 10 \). Moreover, one has \( \dim R(F) \leq 7 \). As each hyperplane of \( \mathcal{H} \) contains infinitely many product vectors, Observation 3 and Proposition 13 imply that \( F \) is not maximal.

**Open problem 3.** Can a maximal face of \( S_1 \) be a polytope?

The next lemma follows easily from [11, Theorem 4].

**Lemma 14** Let \( |a⟩ = |a_1, \ldots, a_n⟩ \) and \( |b⟩ = |b_1, \ldots, b_n⟩ \) be non-parallel product vectors with \( ||a_i|| = ||b_i|| = 1 \) for each \( i \), and let \( F \in \mathcal{F} \) be the face generated by \( |a⟩⟨a| \) and \( |b⟩⟨b| \). If the vector \( |a⟩ + |b⟩ \) is entangled, then \( F \) is the straight line segment joining \( |a⟩⟨a| \) and \( |b⟩⟨b| \). Otherwise, there is a unique index \( i \) such that \( |a_i⟩ \) and \( |b_i⟩ \) are non-parallel, and \( F = \{|x⟩⟨x|\} \) where \( |x⟩ = |a_1, \ldots, a_i - 1, x_i, a_{i+1}, \ldots, a_n⟩ \) and \( |x_i⟩ \) runs through all unit vectors in span\{\(a_i, b_i\}\}.
The above lemma implies that \( \dim F > 0 \) for any maximal face \( F \in \mathcal{F} \). This leads to the following problem.

**Open problem 4.** For a fixed quantum system, find the minimum and the maximum of \( \dim F \) over all maximal faces \( F \in \mathcal{F} \). In particular, are there any faces of dimension \( d^2 - 2 \)?

In the bipartite case it is known that there is no face of dimension \( d^2 - 2 \) (see [11]).

It follows from Proposition [13] that the faces constructed in Propositions [9] and [12] are not maximal except in the two-qubit case (see Proposition [20]). Hence, in the case \( d_1 = \cdots = d_n \) the maximum mentioned in the above problem is bigger than the dimension [15].

### 4.1 Maximal faces associated to hyperplanes

The following theorem provides a very rich family of maximal faces of \( \mathcal{S}_1 \), namely the faces \( F_V \) where \( V \subset \mathcal{H} \) is any hyperplane. Recall that if \( V \subset \mathcal{H} \) is a subspace of codimension > 1 then the associated face \( F_V \) is not maximal (see Proposition [13]).

**Theorem 15** For a subspace \( V \subset \mathcal{H} \), the associated face \( F_V \) is maximal if and only if \( V \) is a hyperplane.

**Proof.** In view of Proposition [13] we need only to prove the sufficiency part. For any product vector \( |\alpha\rangle = |a_1, a_2, \ldots, a_n\rangle \) and distinct indexes \( i_1, \ldots, i_s \in \{1, \ldots, n\} \) and any vectors \( |x_{i_k}\rangle \in \mathcal{H}_{i_k} \) we denote by \( \alpha(x_{i_1}, \ldots, x_{i_s}) \) the product vector obtained from \( |\alpha\rangle \) by replacing each \( |a_{i_k}\rangle \) with the corresponding \( |x_{i_k}\rangle \).

Let \( F \in \mathcal{F} \) be such that \( F_V \subset F \). Since this inclusion is strict, we have \( P_F \not\subseteq V \). We claim that for any product vector \( |\alpha\rangle = |a_1, a_2, \ldots, a_n\rangle \in P_F \setminus V \) with \( \|a_1\| = \cdots = \|a_n\| = 1 \), any distinct indexes \( i_1, \ldots, i_s \in \{1, \ldots, n\} \) and any unit vectors \( |x_{i_k}\rangle \in \mathcal{H}_{i_k} \) we have \( \alpha(x_{i_1}, \ldots, x_{i_s}) \in P_F \). The proof will be by induction on \( s = 1, \ldots, n \).

The case \( s = 1 \) is easy. We may assume that \( |x_{i_1}\rangle \) and \( |a_{i_1}\rangle \) are linearly independent. Since \( V \) is a hyperplane there exists a unit vector \( |v_{i_1}\rangle \in \text{span}\{|a_{i_1}\rangle, |x_{i_1}\rangle\} \) such that \( \alpha(v_{i_1}) \in V \). Since both \( |\alpha\rangle \) and \( \alpha(v_{i_1}) \) belong to \( P_F \), Lemma [14] implies that also \( \alpha(x_{i_1}) \in P_F \).

Now assume that the claim is true for some \( s < n \). We set \( |\beta\rangle = \alpha(x_{i_{s+1}}) \). By using the case \( s = 1 \) we have \( |\beta\rangle \in P_F \). If \( |\beta\rangle \notin V \) then the induction hypothesis implies that \( \beta(x_{i_1}, \ldots, x_{i_s}) \in P_F \), i.e., \( \alpha(x_{i_1}, \ldots, x_{i_{s+1}}) \in P_F \). Next assume that \( |\beta\rangle \in V \). Then \( |a_{i_{s+1}}\rangle \) and \( |x_{i_{s+1}}\rangle \) are linearly independent and we denote by \( |y_{i_{s+1}}\rangle \) a unit vector parallel to \( |a_{i_{s+1}}\rangle + |x_{i_{s+1}}\rangle \). Note that \( |\gamma\rangle := \alpha(y_{i_{s+1}}) \in P_F \setminus V \). By the induction hypothesis we have \( \alpha(x_{i_1}, \ldots, x_{i_s}) \in P_F \) as well as \( \gamma(x_{i_1}, \ldots, x_{i_s}) \in P_F \). It follows from Lemma [14] that \( \alpha(x_{i_1}, \ldots, x_{i_s}, x_{i_{s+1}}) \in P_F \). Hence, the claim holds also for \( s + 1 \).

We conclude that the claim is valid for all \( s = 1, \ldots, n \). When \( s = n \), the claim implies that \( F = \mathcal{S}_1 \) and so \( F_V \) must be a maximal face of \( \mathcal{S}_1 \).

Recall that all induced faces of \( \mathcal{S}_1 \) are exposed. Whether this is true for arbitrary faces is apparently not known.

**Open problem 5.** Is every face of \( \mathcal{S}_1 \) exposed?

**Corollary 16** If \( V \subset \mathcal{H} \) is a hyperplane then \( P_V \) spans \( V \).

**Proof.** Let \( V' \subset V \) be the subspace spanned by \( P_V \). Then \( F_{V'} = F_V \), and the theorem implies that \( F_{V'} \) is a maximal face. It follows from the theorem that \( V' \) must be a hyperplane, and so \( V' = V \). □

We make two remarks related to this corollary. First, we remark that there exist subspaces of \( \mathcal{H} \) of codimension 2 which are not spanned by product vectors. An example is the subspace spanned by the entangled vector \((|01\rangle + |10\rangle) \otimes |0, \ldots, 0\rangle \) and the \( d - 3 \) basic product vectors \(|i_1, i_2, i_3, \ldots, i_n\rangle\) subject to the condition that \( (i_1, i_2) \notin \{(0, 0), (0, 1), (1, 0)\} \) if \( i_3 = 0, \ldots, i_n = 0 \).
Second, one can view the decomposable vectors in the fermionic space $\wedge^N \mathbb{C}^M$ as the counterparts of product vectors. Recently, it has been shown that there exists a subspace of $\wedge^N \mathbb{C}^M$ of codimension 3 which is not spanned by decomposable $N$-vectors [3 Proposition 14]. In the same reference, it has been proved that when $N = 2$ any subspace of codimension at most two is spanned by decomposable $N$-vectors. Whether this is true for $N > 2$ is still unknown.

An interesting problem is to compute the dimension of the maximal faces $F_V$, where $V$ is a hyperplane. Two ILO-equivalent hyperplanes give rise to maximal faces of the same dimension. Therefore it suffices to consider only the representatives of the ILO-equivalence classes of hyperplanes. If $n = 2$ there are only finitely many equivalence classes. Apart from the bipartite systems, the number of equivalence classes of hyperplanes is finite only in finitely many cases, all of them 3-partite. As a first step, we shall compute the dimension of the maximal face associated to the hyperplane orthogonal to a product vector.

**Proposition 17** If $|\alpha\rangle = |a_1, a_2, \ldots, a_n\rangle \in \mathcal{H}$ is a product vector, then the dimension of the maximal face $F_V$ associated to the hyperplane $V = |\alpha\rangle^\perp$ is given by the formula

$$\text{Dim } F_V = d^2 - 1 - \prod_{i=1}^n (2d_i - 1). \quad (27)$$

**Proof.** Denote by $H_i$ the space of Hermitian operators on $\mathcal{H}_i$. Let $H'_i = \{\rho_i \in H_i : \mathcal{R}(\rho) \perp |a_i\rangle\}$ and let $H''_i = (H'_i)^\perp \subset H_i$. Note that $\text{Dim } H_i = d_i^2$, $\text{Dim } H'_i = (d_i - 1)^2$ and $\text{Dim } H''_i = 2d_i - 1$. A product vector belongs to $V$ if and only if it belongs to one of the subspaces $H_1 \otimes \cdots \otimes H_i-1 \otimes |a_i\rangle^\perp \otimes H_{i+1} \otimes \cdots \otimes \mathcal{H}_n$. It follows that $\text{Dim } F_V = \text{Dim } L - 1$ where $L = \sum_{i=1}^n H_1 \otimes \cdots \otimes H_i-1 \otimes H'_i \otimes H_{i+1} \otimes \cdots \otimes \mathcal{H}_n$. This sum is not a direct sum but it may be also written as a direct sum, namely $L = \bigoplus_{i=1}^n H''_i \otimes \cdots \otimes H''_{i-1} \otimes H'_i \otimes H_{i+1} \otimes \cdots \otimes \mathcal{H}_n$. Hence

$$\text{Dim } L = \sum_{i=1}^n \frac{2d_i - 1}{d_i^2} \cdots \frac{2d_{i-1} - 1}{d_{i-1}^2} \left(1 - \frac{2d_i - 1}{d_i^2}\right) d^2$$

$$= d^2 \left(1 - \prod_{i=1}^n \frac{2d_i - 1}{d_i^2}\right) \quad (28)$$

and the formula (27) follows. \hfill \Box

In the bipartite case ($n = 2$), with $d_1 \leq d_2$, there are exactly $d_1$ ILO-equivalence classes of hyperplanes $V \subset \mathcal{H}$. Their representatives are $V_j = |\psi_j\rangle^\perp, j = 1, \ldots, d_1$, where $|\psi_j\rangle \in \mathcal{H}$ is any vector of Schmidt rank $j$, e.g., $|\psi_j\rangle = \sum_{i=1}^j |i, i\rangle$. The dimension of $F_{V_1}$ has been computed in the above proposition. We leave aside the problem of computing in general the dimension of $F_{V_j}$ for $j > 2$. Here we compute $\text{Dim } F_{V_2}$.

**Proposition 18** Let $n = 2$ and $V = |\psi\rangle^\perp$, where $|\psi\rangle \in \mathcal{H}$ is a vector of Schmidt rank 2. Then $\text{Dim } F_V = d(d - 2)$.

**Proof.** We may assume that $|\psi\rangle = |0, 1\rangle - |1, 0\rangle$. We denote by $S_i$ ($i = 1, 2$) the subspace of $\mathcal{H}_i$ spanned by the first two basis vectors $|0\rangle$ and $|1\rangle$. We also set $W_i = S_i^\perp \subset \mathcal{H}_i$. For convenience, we shall identify $S_1$ and $S_2$ and denote this space by $S$. Then any product vector in $V$ can be written as $(t_1 |x\rangle + |z\rangle) \otimes (t_2 |x\rangle + |y\rangle)$, where $|x\rangle \in S, |z\rangle \in W_1, |y\rangle \in W_2$ and $t_i$ are real. Let $L \subseteq H$ be the subspace spanned by all product states $(t_1 |x\rangle + |z\rangle)(t_1 |x\rangle + |z\rangle) \otimes (t_2 |x\rangle + |y\rangle)(t_2 |x\rangle + |y\rangle)$. As $t_i$ are real parameters, $L$ is spanned by all Hermitian matrices of the following nine types:
1) $|x⟩⟨x| \otimes |x⟩⟨x|$, 
2) $(|x⟩⟨z| + |z⟩⟨x|) \otimes |x⟩⟨x|$, 
3) $|x⟩⟨x| \otimes (|x⟩⟨y| + |y⟩⟨x|)$, 
4) $(|x⟩⟨z| + |z⟩⟨x|) \otimes (|x⟩⟨y| + |y⟩⟨x|)$, 
5) $|z⟩⟨z| \otimes |y⟩⟨y|$, 
6) $|z⟩⟨z| \otimes |x⟩⟨x|$, 
7) $|x⟩⟨x| \otimes |y⟩⟨y|$, 
8) $(|x⟩⟨z| + |z⟩⟨x|) \otimes |y⟩⟨y|$, 
9) $|z⟩⟨z| \otimes (|x⟩⟨y| + |y⟩⟨x|)$.

Thus, $L = \bigoplus_{i=1}^{9} L_i$ where $L_i$ is the subspace spanned by the matrices of type $i)$. We have $\text{Dim } L_1 = 9$, $\text{Dim } L_5 = (d_1 - 2)^2(d_2 - 2)^2$, $\text{Dim } L_6 = 4(d_1 - 2)^2$, $\text{Dim } L_7 = 4(d_2 - 2)^2$, $\text{Dim } L_8 = 4(d_1 - 2)(d_2 - 2)^2$ and $\text{Dim } L_9 = 4(d_1 - 2)^2(d_2 - 2)$. It remains to show that $\text{Dim } L_2 = 12(d_1 - 2)$, $\text{Dim } L_3 = 12(d_2 - 2)$ and $\text{Dim } L_4 = 14(d_1 - 2)(d_2 - 2)$. These three proofs use the same arguments and we shall prove only that $\text{Dim } L_4 = 14(d_1 - 2)(d_2 - 2)$.

$H$ is a real subspace of the complex vector space $M$ of all $d \times d$ matrices. Let $T$ be the real subspace of $M$ consisting of all upper triangular matrices with real diagonal elements. The map $H \rightarrow T$ which sends a Hermitian matrix to its upper triangular part is an isomorphism of real vector spaces. Denote by $L'_4$ the image of $L_4$ by this isomorphism. Let us write $|x⟩ = \sum_{j \in \{0, 1\}} \xi_j |j⟩$, $|z⟩ = \sum_{1 \leq l \leq d_1} \xi_l |l⟩$ and $|y⟩ = \sum_{1 \leq k \leq d_2} \eta_k |k⟩$. Then

\[
(|x⟩⟨z| + |z⟩⟨x|) \otimes (|x⟩⟨y| + |y⟩⟨x|) = \sum (\xi_j \xi_r^* \xi_k \eta_k^* |j⟩⟨l| \otimes |r⟩⟨k| + \xi_j \xi_r^* \xi_k \eta_k^* |j⟩⟨l| \otimes |k⟩⟨r|) + (\xi_j \xi_r^* \xi_k \eta_k^* |l⟩⟨j| \otimes |r⟩⟨k| + \xi_j \xi_r^* \xi_k \eta_k^* |l⟩⟨j| \otimes |k⟩⟨r|),
\]

where the summation is over all $j, r \in \{0, 1\}$, $l \in \{2, 3, \ldots, d_1 - 1\}$, and $k \in \{2, 3, \ldots, d_2 - 1\}$. Thus, $L'_4$ is the real subspace of $T$ spanned by all matrices

\[
\sum_{j,r=0}^{1} \sum_{l=2}^{d_1-2} \sum_{k=2}^{d_2-1} (\xi_j \xi_r^* \xi_k \eta_k^* |j⟩⟨l| \otimes |r⟩⟨k| + \xi_j \xi_r^* \xi_k \eta_k^* |j⟩⟨l| \otimes |k⟩⟨r|).
\]

This sum has $8(d_1 - 2)(d_2 - 2)$ terms but only $7(d_1 - 2)(d_2 - 2)$ different monomials occur. By Lemma 7 these monomials are linearly independent over complex numbers. Since each of them takes real as well as imaginary values, it follows from Corollary 8 that $\text{Dim } L_4 = \text{Dim } L'_4 = 14(d_1 - 2)(d_2 - 2)$. This completes the proof.

In the remainder of this section we shall consider in more details two low-dimensional systems.

### 4.2 Two-qubit system

We consider here the two-qubit system only. Note that in this case we have $S = P$ as well as $S_1 = P_1$. The faces of $P$ were classified in [12]. Their classification relies on the previous work [2] where the faces of the cone of positive maps on the algebra of complex $2 \times 2$ matrices were classified. It was observed in [24] that some maximal faces have dimension 8. We present here a new and simple method to classify the maximal faces of $S_1$ up to the $\circ$-action. This agrees with the classification in [12]. Let us start with the description, in the case of two qubits, of the face $F$ constructed in Proposition 9.

**Example 19** Let $V \subset \mathcal{H}$ be the hyperplane consisting of all symmetric tensors in $\mathcal{H}$. The set $P_V$ consists of all product vectors $|x, x⟩$ with $||x|| = 1$. The associated face $F_V$ is the convex hull of all $|z⟩⟨z|$...
with $|z\rangle \in P_V$. Explicitly, this face consists of all positive semidefinite matrices
\[
\begin{bmatrix}
a & x & x & z \\
x^* & b & x & y \\
x^* & b & b & y \\
z^* & y^* & y^* & c
\end{bmatrix}, \quad a + 2b + c = 1. \tag{31}
\]

Obviously, $\dim F_V = 8$ and $F_V$ is not a polytope. By Theorem 15 it is a maximal face of $S_1$. By Proposition 9, the extreme points of $F_V$ are the matrices
\[
\begin{bmatrix}
|\xi|^4 & |\xi|^2\xi^* & |\xi|^2\xi^* & (\xi^*)^2 \\
|\xi|^2\xi^* & |\xi|^2 & |\xi|^2 & |\eta|^2\xi^* \\
|\xi|^2\xi^* & |\xi|^2 & |\xi|^2 & |\eta|^2\xi^* \\
(\xi^*)^2 & |\eta|^2\xi^* & |\eta|^2\xi^* & |\eta|^4
\end{bmatrix}, \quad |\xi|^2 + |\eta|^2 = 1. \tag{32}
\]

The face $F = F^1_V$ is still maximal. It is easy to verify that almost all $\rho \in F$ have full rank, and so we have $\mathcal{R}(F) = \mathcal{H}$.

We can now determine all maximal faces of $S_1$.

**Proposition 20** In the case of two qubits, there are only three GL-equivalence classes of maximal faces of $S_1$. Their representatives are: $F_{V_1}$, $F_{V_2}$, $F^1_{V_2}$, where $V_1 = |0\rangle \otimes \mathcal{H}_2 + \mathcal{H}_1 \otimes |0\rangle$ and $V_2$ is the space of symmetric tensors in $\mathcal{H}$.

**Proof.** It follows from Theorem 15 that the three representatives are indeed maximal faces. Let $F$ be any maximal face. It follows from Proposition 13 that both $\mathcal{R}(F)$ and $\mathcal{R}(F^1)$ have dimension at least $d - 1 = 3$. Assume that both dimensions are 4. Then there exist $\rho_1, \rho_2 \in F$ such that both $\rho_1$ and $\rho_2^1$ have rank 4. Hence the state $(\rho_1 + \rho_2)/2 \in F$ is a full state on $\partial S$. However, we have shown that when $d \leq 6$ there are no such states on $\partial S$. This means that at least one of $\mathcal{R}(F)$ and $\mathcal{R}(F^1)$ must have dimension 3. As $\Gamma$ interchanges the faces $F_{V_2}$ and $F^1_{V_2}$, and preserves $F_{V_1}$, we may assume that $V := \mathcal{R}(F)$ has dimension 3. Hence, (26) implies that $F = F_V$. For nonzero $|a\rangle$ we have $V \cap (|a\rangle \otimes \mathcal{H}_2) \neq 0$. If $|a\rangle \otimes \mathcal{H}_2 \subseteq V$ for some nonzero $|a\rangle$, then it is easy to show that $V$ is GL-equivalent to $V_1$. It follows that $F$ is GL-equivalent to $F_{V_1}$. If there is no such $|a\rangle$, then there is an $A \in \text{GL}$ such that $AV$ is the space of symmetric tensors. Hence, $F$ must be GL-equivalent to $F_{V_2}$ and our claim is proved.

Note that $\dim F_{V_1} = 6$ and $\dim F_{V_2} = 8$ and so we have the following corollary.

**Corollary 21** In $2 \otimes 2$, the minimum and the maximum of $\dim F$ over all maximal faces $F$ is 6 and 8, respectively.

### 4.3 Qubit-qutrit system

In this section we describe the maximal faces of $S_1$ in the $2 \otimes 3$ system. As a byproduct, we obtain that the maximum dimension of the proper faces is 24.

**Proposition 22** In the qubit-qutrit system, there are only three GL-equivalence classes of maximal faces of $S_1$. Their representatives are: $F_{V_1}$, $F_{V_2}$, $F^1_{V_2}$, where $V_1 = |0, 0\rangle^\perp$ and $V_2 = (|0, 2\rangle - |1, 0\rangle)^\perp$. 

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Proof. It follows from Theorem 13 that the three representatives are indeed maximal faces. Let $F$ be any maximal face. It follows from Proposition 13 that both $V := R(F)$ and $R(F^{\Gamma_1})$ have dimension at least $d - 1 = 5$. The case where both dimensions are 6 can be ruled out by the same argument as in the two-qubit case. Thus at least one of $R(F)$ and $R(F^{\Gamma_1})$ must have dimension 5. As $\Gamma_1$ fixes $F_{V_1}$ and interchanges $F_{V_2}$ and $F_{V_1}^{\Gamma_1}$, we may assume that $\dim V = 5$. As $F$ is maximal, (6) implies that $F = F_V$. Note that $\dim V \cap (|a\rangle \otimes \mathcal{H}_2) \geq 2$ for any $|a\rangle \neq 0$.

Assume first that there is a nonzero vector $|a\rangle$ such that $|a\rangle \otimes \mathcal{H}_2 \subset V$. Then there exists $A \in \text{GL}$ such that $AV = V$, and so $F$ is GL-equivalent to $F_{V_1}$. From now on we assume that $|a\rangle \otimes \mathcal{H}_2 \not\subset V$ for all $|a\rangle \neq 0$, and so $\dim V \cap (|a\rangle \otimes \mathcal{H}_2) = 2$. One can easily show that there is a basis $\{|a_i\rangle : i = 0, 1\}$ of $\mathcal{H}_2$ such that $\dim V$ is spanned by the product vectors $|a_0, b_0\rangle$, $|a_0, b_1\rangle$, $|a_1, b_1\rangle$, $|a_1, b_2\rangle$, and $|a, b\rangle$ where $|a\rangle = |a_0\rangle + |a_1\rangle$ and $|b\rangle = |b_0\rangle + |b_1\rangle + |b_2\rangle$. Consequently, there exists $A \in \text{GL}$ such that $AV = V_2$ and we obtain that $F$ is GL-equivalent to $F_{V_2}$.

Since $F_{V_1}$ is GL-equivalent $F_{V_1}^{\Gamma_1}$, it is clear that $F_{V_1}$ is GL-equivalent to neither $F_{V_2}$ nor $F_{V_2}^{\Gamma_1}$. One can verify that $\mathcal{H}_{F_{V_1}^{\Gamma_1}} = \mathcal{H}$. Hence, $F_{V_2}$ is not GL-equivalent to $F_{V_2}$. \hfill \Box

Corollary 23 In $2 \otimes 3$, the minimum and the maximum of $\dim F$ over all maximal faces $F$ is 20 and 24, respectively.

Proof. It suffices to observe that $\dim F_{V_1} = 20$ by Proposition 17 and $\dim F_{V_2} = 24$ by Proposition 18. \hfill \Box

From these results we have the following observation.

Proposition 24 Each maximal face of $S_1$ (of any multipartite quantum system) has dimension at least 6. This lower bound is saturated in the case of two qubits.

Proof. Suppose there is a maximal face $F$ of dimension $< 6$. It follows from Proposition 13 that $\dim F \geq d - 2$, and so $d \leq 7$. As $n > 1$ and each $d_i > 1$, we have $n = 2$ and we may assume that $d_1 = 2$ and $d_2 = 2, 3$. As we have computed the dimensions of the maximal faces in these two cases, we deduce that this is impossible. Thus the first assertion holds. For the second assertion see subsection 4.2. \hfill \Box

5 Some EW for two qutrits

In this section we study the remarkable family of faces $\Delta_b$ of $S_1$ in the two-qutrit quantum system, depending on the parameter $b > 0$, $b \neq 1$. This family was constructed by Ha and Kye in [15]. We have mentioned this family in Example 4 and referred to it already several times. In particular, we have shown in that example that the above faces $\Delta_b$ are not induced. We point out that the very recent paper [14], p. 14, by the same authors, contains another family of faces in $3 \otimes 3$ having similar properties and depending on two real parameters. We shall consider only the one-parameter family in this section. We shall include in our treatement the three limiting cases $b = 0, 1, \infty$.

5.1 A cyclic inequality

The following inequality plays a crucial role in the proof of the main result of this section, Proposition 27.
Lemma 25 Let $a, b > 0$, $c \geq 0$, $a \geq 2(b + c) - 3\sqrt{bc}$ and $(ab - c^2)(ac - b^2) < 0$. Then the homogeneous cyclic inequality

$$\frac{x}{ax + by + cz} + \frac{y}{ay + bz + cx} + \frac{z}{az + bx + cy} \leq \frac{3}{a + b + c}$$

(33)

holds when $x, y, z \geq 0$ and $x + y + z > 0$. The equality sign holds only if (i) $x = y = z$ or at the points (ii) $x = 0$, $bz^2 = cy^2$; (iii) $y = 0$, $bx^2 = cz^2$; (iv) $z = 0$, $by^2 = cx^2$ when $c > 0$ and $a = 2(b + c) - 3\sqrt{bc}$.

Proof. Note that $b \neq c$ because $(ab - c^2)(ac - b^2) < 0$. It is easy to check that

$$2(b + c) - 3\sqrt{bc} > \frac{b^2 + c^2}{b + c},$$

(34)

and so $a(b + c) > b^2 + c^2$. As $(b^2 + c^2)/(b + c) > \sqrt{bc}$, we also have $a^2 > bc$. Let $f(x, y, z)$ denote the function on the left hand side of the inequality (33). We shall first examine the critical points of $f$ in the interior of the first orthant, i.e., when $x, y, z > 0$. The partial derivatives $f_x, f_y, f_z$ of $f$ vanish at a critical point $(x, y, z)$. By taking the linear combinations $bf_y - cf_x$ and $bf_z - cf_y$, we obtain the equations $f_1 f_2 = 0$, $f_3 f_4 = 0$ where

$$f_1 = z(bx - cy) + cx^2 - by^2,$$

(35)

$$f_2 = (a^2 - bc)(bx + cy) + (2abc - b^3 - c^3)z,$$

(36)

$$f_3 = x(by - cz) + cy^2 - bz^2,$$

(37)

$$f_4 = (a^2 - bc)(by + cz) + (2abc - b^3 - c^3)x.$$

(38)

If $f_1 = 0$ it is easy to verify that $bx - cy \neq 0$, and so $z = (by^2 - cx^2)/(bx - cy)$. If $f_1 = f_3 = 0$ then we also have $x = y = z$ and $f(x, y, z) = 3/(a + b + c)$. If $f_1 = f_4 = 0$ we obtain that $y(ab - c^2) = x(ac - b^2)$ and

$$\frac{3}{a + b + c} - f(x, y, z) = \frac{-(a(b + c) - (b^2 + c^2)^3}{(a + b + c)(ab - c^2)(ac - b^2)(a^2 + b^2 + c^2 - ab - ac - bc)} > 0.$$  

(39)

If $f_2 = 0$ then we can solve this equation for $x$. We must have $f_3 = 0$ or $f_4 = 0$. In both cases we obtain again that (33) holds.

It remains to consider the boundary of the first orthant. The inequality holds strictly if two of the variables $x, y, z$ vanish. For instance, if $y = z = 0$ then $a \geq (b^2 + c^2)/(b + c) > (b + c)/2$ because $b \neq c$.

Assume that only $z = 0$. The inequality holds strictly if $c = 0$. Otherwise we have $f(x, y, 0) = g(t) = (c + 2at + bt^2)/((a + bt)(c + at))$ where $t = y/x$. The function $g(t)$ has a maximum at $t = \sqrt{c/b}$ and at that point we have

$$\frac{3}{a + b + c} - g \left( \frac{\sqrt{c}}{\sqrt{b}} \right) = \frac{a - 2(b + c) + 3\sqrt{bc}}{(a + b + c)(a + \sqrt{bc})} \geq 0.$$  

(40)

Thus, the equality sign holds in (33) only if $c > 0$, $a = 2(b + c) - 3\sqrt{bc}$ and $by^2 = cx^2$.

The other two cases can be treated similarly. \hfill \Box

5.2 Entanglement witnesses

Let us recall the definition of (optimal) entanglement witnesses in the bipartite case.
Definition 26 A Hermitian operator $W \in H$ is an entanglement witness (EW) if it satisfies the following two conditions

(i) $W$ has at least one negative eigenvalue;
(ii) $\text{Tr}(W \rho) \geq 0$ for all $\rho \in S_1$.

Thus, if $\rho \in D_1$ and $\text{Tr}(W \rho) < 0$ then $\rho$ is an entangled state. An entanglement witness $W$ is an optimal entanglement witness (OEW) if the set of entangled states detected by $W$ is maximal, i.e.,

(iii) there is no entanglement witness $W'$ such that $\{ \rho \in D_1 : \text{Tr}(W' \rho) < 0 \}$ is a proper subset of $\{ \rho \in D_1 : \text{Tr}(W' \rho) < 0 \}$.

We say that an EW, say $W$, has the spanning property if $\mathcal{H}$ is spanned by the product vectors $|z\rangle$ such that $\text{Tr}(W|z\rangle\langle z|) = 0$. It is a well known fact (see [26, Corollary 2]) that an EW satisfying the spanning property is optimal. This is a sufficient but not necessary condition for optimality. On the other hand, a necessary and sufficient condition for optimality says that an EW $W$ is optimal if and only if $W - P$ is not an EW for any nonzero positive semidefinite matrix $P$ (see [26, Theorem 1]). We will use both criteria in the sequel. If $W$ is an EW, then the condition (ii) implies that $F_W$ is a proper exposed face of $S_1$. If $W$ is an OEW, then the face $F_W$ is nonempty.

From now until the end of this section we consider only the quantum system $3 \otimes 3$. Let us introduce a 1-parameter family $\{W_b\}, b \in [0, \infty]$, of normalized (i.e., with trace 1) Hermitian operators. It is given by the formula

$$W_b = \frac{1}{4} I_9 - \frac{(1 + b)^2}{12(1 - b + b^2)} \sum_{i=1}^{6} |z_i\rangle\langle z_i| - \frac{3(1 - 3b + 2b^2)}{16(1 - b + b^2)} \sum_{i=7}^{10} |z_i\rangle\langle z_i|,$$

where the $|z_i\rangle$ are the normalized product vectors from [15, p. 17]. For $i = 1, 3, 5$ these product vectors are given by

$$|z_1\rangle = (|0\rangle + \sqrt{b}|1\rangle) \otimes (\sqrt{b}|0\rangle + |1\rangle)/(1 + b),$$
$$|z_3\rangle = (|1\rangle + \sqrt{b}|2\rangle) \otimes (\sqrt{b}|1\rangle + |2\rangle)/(1 + b),$$
$$|z_5\rangle = (|2\rangle + \sqrt{b}|0\rangle) \otimes (\sqrt{b}|2\rangle + |0\rangle)/(1 + b).$$

For $i = 2, 4, 6$ they are given by the same formulas except that one should replace $\sqrt{b}$ with $-\sqrt{b}$. The remaining four are

$$|z_7\rangle = (|0\rangle + |1\rangle + |2\rangle) \otimes (|0\rangle + |1\rangle + |2\rangle)/3,$$
$$|z_8\rangle = (|0\rangle + |1\rangle - |2\rangle) \otimes (|0\rangle + |1\rangle - |2\rangle)/3,$$
$$|z_9\rangle = (|0\rangle - |1\rangle + |2\rangle) \otimes (|0\rangle - |1\rangle + |2\rangle)/3,$$
$$|z_{10}\rangle = (-|0\rangle + |1\rangle + |2\rangle) \otimes (-|0\rangle + |1\rangle + |2\rangle)/3.$$

By definition, $W_\infty = \lim_{b \to \infty} W_b$. In order to simplify notation, we have supressed the fact that the $|z_i\rangle$ for $i \leq 6$ depend on the parameter $b$. We shall write $X_b$ for the hyperplane $X_{W_b}$.

We denote by $\Delta_b$ the convex hull of the ten states $|z_i\rangle\langle z_i|$. When $b \neq 0, \infty$, one can easily verify that the ten states $|z_i\rangle\langle z_i|$ are linearly independent and so $\Delta_b$ is a 9-dimensional simplex. In the two exceptional cases, $b = 0, \infty$, we have $|z_i\rangle = |z_{i+1}\rangle$ for $i = 1, 3, 5$ and $\Delta_b$ becomes a 6-dimensional simplex.

For $b \neq 0, 1, \infty$, it was shown in [15] that $\Delta_b$ is a face of $S_1$. In the next proposition we show that all $W_b$ are EW (they are OEW for $b \neq 1$), and we shall write $F_b$ for the face $F_{W_b}$. We will show that $F_b = \Delta_b$ for $b \neq 1$. In particular we obtain another proof of the result mentioned above.
Proposition 27  Let $W_b, X_b, F_b$, and the $|z_i\rangle$ be as defined above.

(i) If $b \neq 0, 1, \infty$ then $W_b$ is an OEW, $F_b = \Delta_b$, and $W_b$ has the spanning property.

(ii) For $b = 1$, $W_1$ is a non-optimal EW and $F_1$ is the convex hull of all states $|x,x\rangle|x,x|$ with real $|x\rangle \in \mathcal{H}_1$ and $\|x\| = 1$.

(iii) If $b = 0, \infty$, then $W_b$ is an OEW, $F_b = \Delta_b$, but $W_b$ lacks the spanning property.

Proof. (i) The characteristic polynomial of $W_b$ has the factorization

$$2^{-8}(t + b)(2t - 3 + 5b - 3b^2)^2 \left(4t^2 - 4(1 + b^2)t - 1 + 2b + b^2 + 2b^3 - b^4\right)^3.$$ (49)

Thus $-b$ is a negative eigenvalue of $W_b$ and so the condition (i) of Def. 26 is satisfied. In order to verify the condition (ii) of the same definition, it suffices to prove that the inequality $\text{Tr}(W_b\rho) \geq 0$ holds for all pure product states $\rho = |x,y\rangle\langle x,y|, |x\rangle = \sum_i x_i|i\rangle \in \mathcal{H}_1$ and $|y\rangle = \sum_i y_i|i\rangle \in \mathcal{H}_2$. A computation gives

$$6(1 - b + b^2)\text{Tr}(W_b\rho) = (1 - b)^2 \sum_i |x_i y_i|^2 + b^2 \sum_i |x_i y_{i+1}|^2 + \sum_i |x_i y_{i-1}|^2 - 2(1 - b + b^2) \sum_i \Re(x_i^* x_{i+1})\Re(y_i^* y_{i+1}).$$ (50)

For convenience, the subscript $i$ runs through integers modulo 3 and we shall use this convention in the rest of this proof. Thus, we have to show that the bihermitian form in the variables $x_i$ and $y_i$ on the right hand side is positive semidefinite. We can view this form as a hermitian form in the $y_i$. Then our task reduces to showing that the matrix of this hermitian form is positive semidefinite, i.e.,

$$X(b) := \begin{bmatrix} p_0 & 0 & 0 \\
0 & p_1 & 0 \\
0 & 0 & p_2 \end{bmatrix} - \frac{1 - b + b^2}{2} (|x\rangle\langle x| + |x^*\rangle\langle x^*|) \geq 0,$$ (51)

where $p_i = (2 - 3b + 2b^2)|x_i|^2 + |x_{i+1}|^2 + b^2|y_i|^2 > 0$. This matrix inequality can be re-written as

$$P^{-1/2}|x\rangle\langle x|P^{-1/2} + P^{-1/2}|x^*\rangle\langle x^*|P^{-1/2} \leq \frac{2}{1 - b + b^2} I_3,$$ (52)

where $P = \text{diag}(p_0, p_1, p_2)$. Since $\langle x^*\rangle P^{-1/2} = \langle x\rangle P^{-1/2} = \sum_i |x_i|^2/p_i$, it suffices to prove that

$$\frac{|x_0|^2}{p_0} + \frac{|x_1|^2}{p_1} + \frac{|x_2|^2}{p_2} \leq \frac{1}{1 - b + b^2}.$$ (53)

It is straightforward to verify that this inequality follows from Lemma 25. (The $a, b, c, x, y, z$ of this lemma should be set to $2 - 3b + 2b^2, 1, b^2, |x_0|^2, |x_1|^2, |x_2|^2$, respectively.) Thus we have shown that $W_b$ is an EW. As $\text{Tr}(W_b|z_i\rangle\langle z_i|) = 0$ for $i = 1, \ldots, 10$, and the $|z_i\rangle$ span $\mathcal{H}$, we conclude that $W_b$ has the spanning property and so it is an OEW.

In order to prove that $F_b = \Delta_b$, it suffices to show that $\text{Tr}(W_b|x,y\rangle\langle x,y|) = 0$ implies that $|x,y\rangle \propto |z_i\rangle$ for some $1 \leq i \leq 10$. Thus, let us assume that $\text{Tr}(W_b|x,y\rangle\langle x,y|) = 0$. Then the equality sign must hold in the inequality (53). By Lemma 25, there are four possibilities.

First, the $x_i$ have the same modulus, say 1. We can assume that $x_0 = 1, x_1 = e^{i\alpha}, x_2 = e^{i\beta}$ with $\alpha, \beta \in \mathbb{R}$. By plugging these values into $X(b)$, we find that

$$\det X(b) = 6(1 - b + b^2)^3(3 - \cos 2\alpha - \cos 2\beta - \cos 2(\alpha - \beta)).$$

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As $X(b)$ must be singular, we deduce that $\cos 2\alpha = \cos 2\beta = \cos 2(\alpha - \beta) = 1$. Thus we obtain that $x_1 = \pm 1$ and $x_2 = \pm 1$. In each of these four subcases $X(b)$ has rank 2 and so there is (up to a scalar factor) a unique vector $|y\rangle$ such that $X(b)|y\rangle = 0$. Therefore $|x, y\rangle \propto |z_i\rangle$ for some $i = 7, \ldots, 10$.

Second, $x_0 = 0$ and $|x_2|^2 = b|x_1|^2$. We may assume that $x_1 = 1$ and so $|x_2| = \sqrt{b}$. Since $X(b)$ must be a singular matrix, we obtain that $x_2 = \pm \sqrt{b}$. This leads to the solutions $|z_3\rangle$ and $|z_4\rangle$.

The remaining two cases are similar to the last one. Thus, we have shown that $F_b = \Delta_b$.

(ii) Let $|x, y\rangle \in \mathcal{H}$ be an arbitrary unit product vector. Then one can verify that

$$12 \langle x, y|W_1|x, y\rangle = |x_0y_1 - x_1y_0|^2 + |x_0y_2 - x_2y_0|^2 + |x_1y_2 - x_2y_1|^2 + |x_0y_1^* - x_1y_0^*|^2 + |x_0y_2^* - x_2y_0^*|^2 + |x_1y_2^* - x_2y_1^*|^2,$$

where $x_i$ and $y_i$ are the components of $|x\rangle$ and $|y\rangle$, respectively. It follows that $W_1$ is an EW and that $F_1$ is indeed the convex hull of the set of pure product states $|x, x\rangle|x, x\rangle$ with real $|x\rangle \in \mathcal{H}_1$ and $\|x\| = 1$. However, $W_1$ is not an OEW. Indeed, if $|e_{ij}\rangle = |ij\rangle - |ji\rangle$, then one can easily verify that

$$W := 2W_1 - \frac{1}{6} \sum_{0 \leq i < j < 3} |e_{ij}\rangle\langle e_{ij}|$$

$$= \frac{1}{6} \left( I_3 - \sum_{i,j=0}^2 |ii\rangle\langle jj| \right)$$

is an EW.

(iii) We give the proof only when $b = 0$. The case $b = \infty$ can be treated similarly. (Note that $W_b = W_{1/b}$ for all $b \in [0, \infty]$ and that $|z_i(1/b)\rangle$ is obtained from $|z_i(b)\rangle$ by switching $\mathcal{H}_1$ and $\mathcal{H}_2$.) By setting $b = 0$ in Eq. (49) we infer that $W_0$ has a negative eigenvalue, namely $(1 - \sqrt{2})/2$. By using the continuity of the map sending $b \to W_b$, we deduce that $W_0$ is an EW. To prove the optimality, we need to show that $W_0 - P$ is not an EW for any nonzero $P \geq 0$ [20]. Since the product states $|z_i\rangle|z_i\rangle \in X_0$, we may assume that $P|z_i\rangle = 0$. Thus, $\mathcal{R}(P) \subseteq \text{span}\{|\alpha\rangle, |\beta\rangle\}$ where $|\alpha\rangle = |00\rangle - |11\rangle$ and $|\beta\rangle = |11\rangle - |22\rangle$. We have $P = |p\alpha + q\beta\rangle\langle p\alpha + q\beta| + |r\alpha + s\beta\rangle\langle r\alpha + s\beta|$, where $p, r \geq 0$ and $q, s$ are some complex numbers. By a straightforward computation, for any $b > 0$ we have $\langle z_i|W_0 - P|z_i\rangle = -b(|q|^2 + |s|^2 - b/6)/(1 + b)^2$ and $\langle z_3|W_0 - P|z_3\rangle = -b(p^2 + r^2 - b/6)/(1 + b)^2$. Hence, at least one of these expressions is negative for small $b > 0$. We conclude that $W_0$ is an OEW.

Next we show that $W_0$ violates the spanning property. Since $b = 0$, we have $|z_i\rangle = |z_{i+1}\rangle$ for $i = 1, 3, 5$. Hence, it suffices to show that if $|z\rangle = |x, y\rangle$ and $\langle z|W_0|z\rangle = 0$ then $|z\rangle \propto |z_i\rangle$ for some $i$. If a component of $|x\rangle$ or $|y\rangle$ vanishes, we claim that $|z\rangle \propto |z_i\rangle$ for some $i \in \{1, 3, 5\}$. Say $x_0 = 0$, then (50) with $b = 0$ can be rewritten as $|x_1y_1 - x_2y_2|^2 + |x_1y_1 - x_2y_2|^2 + 2|x_1y_0|^2 + 2|x_2y_1|^2 = 0$. It follows that $|z\rangle \propto |z_3\rangle$ or $|z\rangle \propto |z_5\rangle$. This proves our claim. Assume now that no component of $|x\rangle$ or $|y\rangle$ vanishes. Let $|x'\rangle \in \mathcal{H}_1$ be the vector having components $|x_i\rangle$, and define $|y'\rangle \in \mathcal{H}_2$ similarly. We also set $|z'\rangle = |x', y'\rangle$. By setting $b = 0$ in (50) and by using the fact that $W_0$ is an EW, we obtain that

$$0 = 6\langle z|W_0|z\rangle \geq \sum_i |x_iy_i|^2 + \sum_i |x_iy_{i-1}|^2 - 2\sum_i |x_ix_{i+1}y_{i+1}| = 6\langle z'|W_0|z'\rangle \geq 0.$$ 

It follows that $|x_ix_{i+1}y_{i+1}| = \mathcal{R}(x_i^*x_{i+1})\mathcal{R}(y_i^*y_{i+1})$ for $i = 0, 1, 2$. Since no component of $|x\rangle$ or $|y\rangle$ vanishes, both $x_i^*x_{i+1}$ and $y_i^*y_{i+1}$ are real. Without any loss of generality we may assume that all $x_i$ and $y_i$ are real. Moreover, we may assume that $x_0 > 0$, $y_0 > 0$, $x_1y_1 > 0$ and $x_2y_2 > 0$. Define the matrix $X(0)$ by setting $b = 0$ in (51). It was shown in the proof of part (i) that $X(b) \geq 0$ for $b > 0$. By continuity, we also have $X(0) \geq 0$. An easy computation gives $\langle y|X(0)|y\rangle = 6\langle z|W_0|z\rangle = 0$. As $|y\rangle \neq 0$,
it follows that \( \det X(0) = 0 \). Equivalently, when \( b = 0 \) then the equality holds in (53). By applying Lemma 25 and assuming that \( \|x\| = \|y\| = 1 \), we obtain that \( x_0^2 = x_1^2 = x_2^2 = 1/3 \). It follows easily that \( |z\rangle \propto |z_i\rangle \) for some \( i \in \{7, 8, 9, 10\} \). This completes the proof.

Let us make a few additional remarks about the faces \( F_b \) in the above proposition. We claim that the faces \( F_0, F_1 \) (and \( F_\infty \)) are not induced. If we set \( n = 2 \) and \( d_1 = d_2 = 3 \) in Proposition 12, then \( F' = F_1 \), and so \( F_1 \) is not induced. The proof for \( F_0 \) is similar to the proof of part (iii) of the mentioned proposition. It uses the facts that the subspace \( \mathcal{R}(F_0) \) is spanned by 7 linearly independent real product vectors and that this subspace contains infinitely many product vectors. By Proposition 13 the faces \( F_0, F_1, F_\infty \) are not maximal. For other faces \( F_b \) see the example below that proposition.

**Corollary 28** When \( d_1 = d_2 = 3 \) then the set of normalized OEW is not closed.

**Proof.** It suffices to note that \( W_1 \) is the limit of the sequence \( W_{1+1/m} \) as \( m \to \infty \).

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