

## On extremal quantum states of composite systems with fixed marginals

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We study the convex set  $\mathcal{C}(\rho_1, \rho_2)$  of all bipartite quantum states with fixed marginal states  $\rho_1$  and  $\rho_2$ . The extremal states in this set have recently been characterized by Parthasarathy [Ann. Henri Poincaré (to appear), quant-ph/0307182]. Here we present an alternative necessary and sufficient condition for a state in  $\mathcal{C}(\rho_1, \rho_2)$  to be extremal. Our approach is based on a canonical duality between bipartite states and a certain class of completely positive maps and has the advantage that it is easier to check and to construct explicit examples of extremal states. In dimension  $2 \times 2$  we give a simple new proof for the fact that all extremal states in  $\mathcal{C}(\frac{1}{2}\mathbb{1}, \frac{1}{2}\mathbb{1})$  are precisely the projectors onto maximally entangled wave functions. We also prove that in higher dimension this does not hold and construct an explicit example of an extremal state in  $\mathcal{C}(\frac{1}{3}\mathbb{1}, \frac{1}{3}\mathbb{1})$  that is not maximally entangled. Generalizations of this result to higher dimensions are also discussed. © 2004 American Institute of Physics. [DOI: 10.1063/1.1776642]

### I. INTRODUCTION

In the paradigmatic situation encountered in quantum information processing, two or more (often spatially separated) parties share the different parts of a composite quantum system. The parties are able to perform arbitrary operations on their respective parts "locally" and to communicate classically among each other to orchestrate their actions. The fundamental realization in quantum information theory is that sharing the parts of a composite quantum system can enable the parties to perform certain communication or information processing tasks more efficiently than classically (see Ref. 1 for an introduction). Mathematically this setting raises a number of new and interesting structural questions. Among them the study of quantum channels and the characterization of quantum entanglement play a central role.<sup>2-4</sup> The present work is devoted to the characterization of the set of quantum states with fixed marginal states. This problem was recently posed and studied in detail by Parthasarathy.<sup>5</sup> Let  $\mathcal{H}_1$  and  $\mathcal{H}_2$  be two finite dimensional complex Hilbert spaces, corresponding to two finite level quantum systems  $S_1$  and  $S_2$ . Without loss of generality we assume that  $d := \dim(\mathcal{H}_1) = \dim(\mathcal{H}_2)$ . (Otherwise we embed the lower dimensional Hilbert space into the larger one.) The states for  $S_i$  are given by the positive operators on  $\mathcal{H}_i$  with trace one. We denote the set of all states on  $\mathcal{H}_i$  by  $\mathcal{S}(\mathcal{H}_i)$ . The composite quantum system  $S_{12}$  of  $S_1$  and  $S_2$  is described by the tensor product  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . A state for  $S_{12}$  is a positive operator on  $\mathcal{H}_1 \otimes \mathcal{H}_2$  with trace one. The space of all states is denoted by  $\mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ . Consider  $\rho \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ . The *reductions* or *marginal states* of  $\rho$  are given by  $\rho_1 := \text{tr}_2(\rho) \in \mathcal{S}(\mathcal{H}_1)$  and  $\rho_2 := \text{tr}_1(\rho) \in \mathcal{S}(\mathcal{H}_2)$ . Here  $\text{tr}_1$  and  $\text{tr}_2$  denote the partial traces over  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , respectively. Now fix  $\rho_1 \in \mathcal{S}(\mathcal{H}_1)$  and  $\rho_2 \in \mathcal{S}(\mathcal{H}_2)$ . We denote by  $\mathcal{C}(\rho_1, \rho_2)$  the convex set of all states  $\rho \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$  whose marginal states are equal to  $\rho_1$  and  $\rho_2$ , respectively. The set of extreme points of  $\mathcal{C}(\rho_1, \rho_2)$  will be denoted by  $\mathcal{E}(\rho_1, \rho_2)$ . Throughout this paper we will denote the set of all operators on a Hilbert space  $\mathcal{H}$  by  $\mathcal{L}(\mathcal{H})$ . The identity in  $\mathcal{L}(\mathcal{H})$  is denoted by  $\mathbb{1}$ , or, when  $\mathcal{H}$  is  $d$ -dimensional, by  $\mathbb{1}_d$ . Slightly abusing the notation we will also denote the identity map from  $\mathcal{L}(\mathcal{H})$  into itself by  $\mathbb{1}$ .

In his work<sup>5</sup> Parthasarathy presented a necessary and sufficient condition for an element  $\rho \in \mathcal{C}(\rho_1, \rho_2)$  to be an extreme point. This was then used to derive an upper bound on the rank of such an extremal state. In the special case  $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$  and  $\rho_1 = \rho_2 = \frac{1}{2}\mathbb{1}_2$ , Parthasarathy found that

a state  $\rho \in \mathcal{C}(\frac{1}{2}\mathbb{1}_2, \frac{1}{2}\mathbb{1}_2)$  is extremal if and only if it is a projector onto the subspace spanned by a maximally entangled wave function. A wave function in  $\mathbb{C}^2 \otimes \mathbb{C}^2$  is called maximally entangled if it is of the form  $|\psi_+\rangle = (1/\sqrt{2})(|0\rangle|\phi_0\rangle + |1\rangle|\phi_1\rangle)$  where  $\{|0\rangle, |1\rangle\}$  denotes the canonical basis of  $\mathbb{C}^2$  and where  $\{|\phi_0\rangle, |\phi_1\rangle\}$  is any other orthonormal basis of  $\mathbb{C}^2$ . For higher dimensions the question of whether or not there are extremal states with maximally mixed marginals—i.e., states in  $\mathcal{E}(\frac{1}{d}\mathbb{1}, \frac{1}{d}\mathbb{1})$ —that are not projectors onto maximally entangled wave functions was left open in Ref. 5.

In the present work we present an alternative approach to the characterization of  $\mathcal{E}(\rho_1, \rho_2)$  that transforms the problem into that of finding the extreme points of a certain convex set of completely positive maps that satisfy an additional requirement. This will allow us to derive an alternative necessary and sufficient condition for a state  $\rho \in \mathcal{C}(\rho_1, \rho_2)$  to be extremal. We will then study the special case of states with maximally mixed marginals, i.e., when  $\rho_1 = \rho_2 = (1/d)\mathbb{1}$ . For  $d=2$  we will give a simple proof for Parthasarathy's result that the extremal states are exactly the projectors onto maximally entangled wave functions. For  $d>2$  our results imply that there are extremal states in  $\mathcal{E}(1/d, 1/d)$  that are not projectors onto maximally entangled pure states. We give an explicit example for an extremal state on  $\mathbb{C}^3 \otimes \mathbb{C}^3$  with maximally mixed marginals that is not equal to a projector onto a maximally entangled wave function. Finally, we discuss generalizations of this result to higher dimensions.

## II. DUALITY BETWEEN BIPARTITE STATES AND COMPLETELY POSITIVE MAPS

The approach in the present paper relies upon a duality between bipartite quantum states on  $\mathcal{H}_1 \otimes \mathcal{H}_2$  and completely positive maps  $\Lambda: \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  that preserve the trace of the completely mixed state, i.e., that satisfy  $\text{tr}(\Lambda((1/d)\mathbb{1}))=1$  (this is very often called the *Jamiołkowski isomorphism*, see Ref. 6 and, for a related duality, Ref. 2). A map  $\Lambda: \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  is called completely positive if  $\Lambda \otimes \mathbb{1}: \mathcal{L}(\mathcal{H}_2 \otimes \mathcal{K}) \rightarrow \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{K})$  is positive for any finite dimensional ancilla Hilbert space  $\mathcal{K}$ .

We make the identification  $\mathcal{H}_1 \simeq \mathbb{C}^d$  and  $\mathcal{H}_2 \simeq \mathbb{C}^d$ . In other words, we pick orthonormal bases in  $\mathcal{H}_1$  and  $\mathcal{H}_2$  and identify them with the canonical real basis in  $\mathbb{C}^d$  and  $\mathbb{C}^d$ , respectively. We denote these bases by  $\{|i\rangle_1\}_{i=1}^d$  and  $\{|i\rangle_2\}_{i=1}^d$ , respectively. Finally, we introduce the maximally entangled pure wave function

$$|\psi_+\rangle := \frac{1}{\sqrt{d}} \sum_{i=1}^d |i\rangle_2 |i\rangle_1 \in \mathcal{H}_2 \otimes \mathcal{H}_1.$$

The duality between bipartite state and completely positive maps depends explicitly on this choice for the canonical bases. Let  $\Lambda: \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  be a completely positive map with  $\text{tr}(\Lambda((1/d)\mathbb{1}))=1$ . Then

$$\rho_\Lambda := \Lambda \otimes \mathbb{1}(|\psi_+\rangle\langle\psi_+|) \quad (1a)$$

defines a bipartite state on  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . The complete positivity of  $\Lambda$  ensures that  $\rho \geq 0$  while the condition  $\text{tr}(\Lambda((1/d)\mathbb{1}))=1$  ensures that  $\text{tr}(\rho_\Lambda)=1$ .

Conversely, let  $\rho$  be a bipartite state on  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . Then

$$\Lambda_\rho(\sigma) := d \text{tr}_2[(\mathbb{1} \otimes \sigma^T \rho)] \quad (1b)$$

defines a completely positive map  $\Lambda_\rho: \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  that satisfies  $\text{tr}(\Lambda_\rho((1/d)\mathbb{1}))=1$ . Here  $^T$  denotes the transposition with respect to the canonical real basis. By explicit calculation one checks that for a given  $\Lambda$  we have  $\Lambda_{\rho_\Lambda} = \Lambda$  and for a given  $\rho$  we have  $\rho_{\Lambda_\rho} = \rho$ . Thus the correspondence  $\Lambda \leftrightarrow \rho$  described by Eqs. (1a) and (1b) is bijective.<sup>6</sup>

### III. JOINT LINEAR INDEPENDENCE

To formulate the main result in this paper it is useful to introduce the concept of *joint linear independence* of two families of vectors. In the following definition  $X^{\times r}$  denotes the  $r$ -fold Cartesian product of the set  $X$  by itself.

*Definition 1:* Let  $V$  and  $W$  be complex vector spaces. Then two ordered  $r$ -tuples  $(v_i)_{i=1}^r \in V^{\times r}$  and  $(w_i)_{i=1}^r \in W^{\times r}$  are called jointly linearly independent if the family  $\{v_i \oplus w_i\}_{i=1}^r$  in the direct sum  $V \oplus W$  is a linearly independent family.

Notice that this definition depends on the order of the  $r$ -tuples. The following is an immediate consequence of the definition.

*Lemma 1:* Let  $V$  and  $W$  be complex vector spaces and let  $(v_i)_{i=1}^r \in V^{\times r}$  and  $(w_i)_{i=1}^r \in W^{\times r}$  be two ordered  $r$ -tuples of vectors. If  $\{v_i\}_{i=1}^r$  is linearly independent in  $V$  or if  $\{w_i\}_{i=1}^r$  is linearly independent in  $W$ , then  $(v_i)_{i=1}^r$  and  $(w_i)_{i=1}^r$  are jointly linearly independent.

Notice that the converse implication does not hold in general. If  $\{v_i\}_{i=1}^r$  is linearly dependent in  $V$  and if  $\{w_i\}_{i=1}^r$  is linearly dependent in  $W$ , then  $\{v_i \oplus w_i\}_{i=1}^r$  is not necessarily linearly dependent in  $V \oplus W$ .

*Lemma 2:* Let  $V$  be a complex  $*$ -algebra and let  $(v_j)_{j=1}^r \in V^{\times r}$  be an ordered  $r$ -tuple of elements. If  $\{v_j\}_j$  is linearly dependent, then the  $r^2$ -tuples  $(v_i^* v_j)_{ij}$  and  $(v_j v_i^*)_{ij}$  cannot be jointly linearly independent.

*Proof:* Since  $\{v_j\}_j$  is linearly dependent, there exist  $(\lambda_j)_j \in \mathbb{C}^r$  such that  $\lambda_{j_0} \neq 0$  for some  $j_0$  and  $\sum_{j=1}^r \lambda_j v_j = 0$ . Therefore also  $\sum_{ij} \delta_{i_0} \lambda_j (v_i^* v_j, v_j v_i^*) = 0$  for all  $i_0$ .  $\square$

### IV. EXTREMAL STATES IN $\mathcal{C}(\rho_1, \rho_2)$

Let  $\rho \in \mathcal{C}(\rho_1, \rho_2)$ . In  $\mathcal{H}_2$  consider an orthonormal basis of eigenvectors of  $\rho_2$ , i.e.,  $\rho_2 = \sum_i r_i |r_i\rangle\langle r_i|$ . We identify the basis  $\{|r_i\rangle\}_{i=1}^d$  of eigenvectors of  $\rho_2$  with the canonical real basis of  $\mathcal{H}_2 \simeq \mathbb{C}^d$ . Further, we write

$$|\psi_+\rangle := \frac{1}{\sqrt{d}} \sum_i |r_i\rangle \otimes |r_i\rangle. \tag{2}$$

In the sequel it is always understood that the bijection between states and completely positive maps from Sec. II is with respect to this choice of the canonical basis and that the maximally entangled state in Eq. (1a) is the state from Eq. (2). To every state  $\rho \in \mathcal{C}(\rho_1, \rho_2)$  Eq. (1b) gives a unique completely positive map  $\Lambda_\rho$  that satisfies

$$\Lambda_\rho(\mathbb{1}) = d\rho_1, \tag{3a}$$

$$\Lambda'_\rho(\mathbb{1}) = d\rho_2. \tag{3b}$$

Here  $\Lambda'_\rho$  denotes the canonical dualization of  $\Lambda_\rho$  defined by  $\text{tr}(\Lambda'_\rho(x)y) = \text{tr}(x\Lambda_\rho(y))$  for all  $y$ . In terms of the Kraus representation of  $\Lambda_\rho(x) = \sum_j V_j^\dagger x V_j$  the conditions (3a) and (3b) can be expressed as

$$\sum_j V_j^\dagger V_j = d\rho_1, \tag{4a}$$

$$\sum_j V_j V_j^\dagger = d\rho_2. \tag{4b}$$

We denote the set of all completely positive maps  $\Lambda : \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  satisfying the conditions (3a) and (3b) by  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$ . It is clear that  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$  is a convex set. The bijection described in (1a) and (1b) obviously respects the convex structure. In particular it establishes a bijection between  $\mathcal{E}(\rho_1, \rho_2)$  and the extreme points of  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$ .

We are now ready to state our main result.

**Theorem 1:** Let  $\Lambda: \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  be a completely positive map in  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$ . Then  $\Lambda$  is extreme in  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$  if and only if  $\Lambda$  admits an expression  $\Lambda(x) = \sum_j V_j^\dagger x V_j$  for all  $x \in \mathcal{L}(\mathcal{H}_2)$ , where  $V_i$  are  $d \times d$  matrices, satisfying the following conditions:

- (i)  $\sum_j V_j^\dagger V_j = d\rho_1$ ,
- (ii)  $\sum_j V_j V_j^\dagger = d\rho_2$ , and
- (iii)  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are jointly linearly independent.

For the proof of Theorem 1 we need the following lemma. For a proof see Remark 4 in Ref. 7.  
**Lemma 3:** Let  $\Lambda$  be a completely positive map with Kraus representation  $\Lambda(x) = \sum_j V_j^\dagger x V_j$  with  $\{V_j\}_j^\ell$  linearly independent. Let  $\{W_p\}_p^{\ell'}$  be a class of  $d \times d$  matrices, then  $\Lambda$  has the expression  $\Lambda(x) = \sum_p W_p^\dagger x W_p$  if and only if there exists an isometric  $\ell' \times \ell$  matrix  $(\mu_{pi})_{pi}$ , such that  $W_p = \sum_i \mu_{pi} V_i$  for all  $p$ .

*Proof of Theorem 1:* The proof is an only slight modification and generalization of the proof of Theorem 5 in Ref. 7. We include it for the convenience of the reader. First assume that  $\Lambda$  is extremal in  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$ . We express  $\Lambda$  in Kraus form  $\Lambda(x) = \sum_j V_j^\dagger x V_j$ . Without loss of generality we can assume that  $\{V_j\}_j$  is linearly independent.<sup>7</sup> Now suppose that  $\sum \lambda_{ij} V_i^\dagger V_j = 0$  and  $\sum_{ij} \lambda_{ij} V_j V_i^\dagger = 0$ . We need to show that  $\lambda_{ij} = 0$ . Without loss of generality we can assume that  $(\lambda_{ij})_{ij}$  is a Hermitian matrix and  $-1 \leq (\lambda_{ij})_{ij} \leq 1$  (for details see Ref. 7).

Define  $\Phi_\pm: \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  by  $\Phi_\pm(x) := \sum_j V_j^\dagger x V_j \pm \sum_{ij} \lambda_{ij} V_i^\dagger x V_j$ . Hence  $\Phi_\pm(1) = d\rho_1$  and  $\Phi_\pm^\dagger(1) = d\rho_2$ . We set  $1 + (\lambda_{ij})_{ij} = (\alpha_{ij})_{ij}^\dagger (\alpha_{ij})_{ij} \geq 0$  and  $W_i := \sum_j \alpha_{ij} V_j$ . By direct computation,  $\Phi_+(x) = \sum_i W_i^\dagger x W_i$ . Hence  $\Phi_+$  is completely positive. Similarly it can be shown that  $\Phi_-$  is completely positive. Since  $\Lambda$  is extremal, we find that  $\Lambda = \Phi_+$ . Therefore by Lemma 3  $(\alpha_{ij})_{ij}$  is an isometry and  $1 + (\lambda_{ij})_{ij} = 1$ . This implies  $(\lambda_{ij})_{ij} = 0$ .

Now assume that  $\Lambda$  admits a representation of the form  $\Lambda(x) = \sum_j V_j^\dagger x V_j$  for all  $x \in \mathcal{L}(\mathcal{H}_2)$  where  $\sum_j V_j^\dagger V_j = d\rho_1$ ,  $\sum_j V_j V_j^\dagger = d\rho_2$ , and  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are jointly linearly independent. By Lemma 2 also  $\{V_j\}_j$  is linearly independent. Now suppose  $\Lambda = \frac{1}{2}(\Phi_1 + \Phi_2)$  with  $\Phi_1(x) = \sum_p W_p^\dagger x W_p$ ,  $\Phi_2(x) = \sum_q Z_q^\dagger x Z_q$ , and  $\sum_p W_p^\dagger W_p = \sum_q Z_q^\dagger Z_q = d\rho_1$ ,  $\sum_p W_p W_p^\dagger = \sum_q Z_q Z_q^\dagger = d\rho_2$ . Since  $\Lambda(x) = \frac{1}{2} \sum_p W_p^\dagger x W_p + \frac{1}{2} \sum_q Z_q^\dagger x Z_q$ , it follows by Lemma 3 that  $W_p$  and  $Z_q$  can be expressed as a linear combination of the  $V_j$ . Let  $W_p = \sum_i \mu_{pi} V_i$  for all  $p$ . Then  $\sum_j V_j^\dagger V_j = \sum_p W_p^\dagger W_p = \sum_{pij} \mu_{pi}^* \mu_{pj} V_i^\dagger V_j$  and  $\sum_j V_j V_j^\dagger = \sum_p W_p W_p^\dagger = \sum_{pij} \mu_{pi} \mu_{pj}^* V_j V_i^\dagger$ . The joint linear independence of  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  implies  $\sum_p \mu_{pi}^* \mu_{pj} = \delta_{ij}$ . In other words  $(\mu_{pi})_{pi}$  is an isometry. By Lemma 3, we conclude that  $\Lambda = \Phi_1$ . Thus  $\Lambda$  is extremal in  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$ .  $\square$

**Corollary 1:** Let  $\rho \in \mathcal{C}(\rho_1, \rho_2)$ . Write the spectral decomposition of  $\rho_2$  as  $\rho_2 = \sum_i r_i |r_i\rangle\langle r_i|$ . Then  $\rho \in \mathcal{E}(\rho_1, \rho_2)$  if and only if there exists a family of  $d \times d$  matrices  $\{V_j\}$  such that  $\rho$  can be expressed as

$$\rho = \frac{1}{d} \sum_{ijk} V_j^\dagger |r_i\rangle\langle r_k| V_j \otimes |r_i\rangle\langle r_k|,$$

where  $\{V_j\}_j$  satisfy the following conditions:

- (i)  $\sum_j V_j^\dagger V_j = d\rho_1$ ,
- (ii)  $\sum_j V_j V_j^\dagger = d\rho_2$ , and
- (iii)  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are jointly linearly independent.

**Remark 1:** Suppose  $\Lambda: \mathcal{L}(\mathcal{H}_2) \rightarrow \mathcal{L}(\mathcal{H}_1)$  is completely positive. Then we can write  $\Lambda(x) = \sum_j V_j^\dagger x V_j$  where  $\{V_j\}_{j=1}^\ell$  is a class of linearly independent  $d \times d$  matrices. Therefore  $\ell \leq d^2$ . If  $\Lambda$  is extremal in  $\text{CP}(\mathcal{H}_2, \mathcal{H}_1, \rho_1, \rho_2)$ , we can conclude that  $\ell \leq \sqrt{2d}$ . Indeed,  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are jointly linearly independent only if the cardinal number of  $\{V_i^\dagger V_j \oplus V_j V_i^\dagger\}_{ij}$  is smaller than  $\dim(\mathcal{L}(\mathcal{H}_2)) + \dim(\mathcal{L}(\mathcal{H}_1))$ . In other words,  $\ell^2 \leq 2d^2$ , i.e.,  $\ell \leq \sqrt{2d}$ . Parthasarathy found a slightly stronger bound in Ref. 5.  $\ell \leq \sqrt{2d^2 - 1}$ . It is not known whether this bound is tight.

**Remark 2:** The bound  $\ell \leq \sqrt{2d}$  also implies that for any  $\rho \in \mathcal{E}(\rho_1, \rho_2)$  we have  $\text{rank}(\rho) \leq \sqrt{2d}$ . In all dimensions  $d \geq 2$  this implies that any  $\rho \in \mathcal{E}(\rho_1, \rho_2)$  is singular.

**V. EXAMPLES**

**A. A two dimensional example**

Consider  $\mathbb{C}^2 \otimes \mathbb{C}^2$  and the convex set  $\mathcal{C}(\frac{1}{2}\mathbb{1}, \frac{1}{2}\mathbb{1})$  of states on  $\mathbb{C}^2 \otimes \mathbb{C}^2$  with maximally mixed marginals. This is a physically interesting example. It was previously studied in Ref. 5.

Assume that  $\rho \in \mathcal{E}(\frac{1}{2}\mathbb{1}, \frac{1}{2}\mathbb{1})$ , i.e., that  $\rho$  is extremal in  $\mathcal{C}(\frac{1}{2}\mathbb{1}, \frac{1}{2}\mathbb{1})$ . By Corollary 1 there is a linearly independent family of  $2 \times 2$  matrices  $\{V_j\}_{j=1}^\ell$  such that

$$\rho = \frac{1}{2} \sum_{ijk} V_j^\dagger |r_i\rangle\langle r_k| V_j \otimes |r_i\rangle\langle r_k|,$$

where  $\{V_j\}$  satisfy the following conditions:

$$\sum_j V_j^\dagger V_j = \mathbb{1}_2, \tag{5a}$$

$$\sum_j V_j V_j^\dagger = \mathbb{1}_2, \tag{5b}$$

and where  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are jointly linearly independent.

By Remark 1 either  $\ell=1$  or  $\ell=2$ . In the case  $\ell=1$ , the matrix  $V_1$  is unitary and it follows from Corollary 1 that  $\rho$  is equal to the projector onto the subspace spanned by a maximally entangled wave function.

Now consider the case  $\ell=2$ . Consider the singular value decompositions of  $V_1$  and  $V_2$ , respectively, i.e.,  $V_1 = \sum_{s=1}^2 \sqrt{\nu_s(1)} |\varphi_s\rangle\langle\psi_s|$  and  $V_2 = \sum_{s=1}^2 \sqrt{\nu_s(2)} |\varphi'_s\rangle\langle\psi'_s|$ , where  $\nu_s(i)$  are non-negative coefficients and where  $\{|\psi_s\rangle\}_{s=1}^2, \{|\psi'_s\rangle\}_{s=1}^2, \{|\varphi_s\rangle\}_{s=1}^2$  and  $\{|\varphi'_s\rangle\}_{s=1}^2$  are four orthonormal bases of  $\mathbb{C}^2$ . Then  $V_1^\dagger V_1 = \sum_{s=1}^2 \nu_s(1) |\psi_s\rangle\langle\psi_s|$ ,  $V_2^\dagger V_2 = \sum_{s=1}^2 \nu_s(2) |\psi'_s\rangle\langle\psi'_s|$ ,  $V_1 V_1^\dagger = \sum_{s=1}^2 \nu_s(1) |\varphi_s\rangle\langle\varphi_s|$  and  $V_2 V_2^\dagger = \sum_{s=1}^2 \nu_s(2) |\varphi'_s\rangle\langle\varphi'_s|$ .

First consider the case of degenerate singular values, i.e., assume  $\nu_1(1) = \nu_2(1)$ . Then  $V_1^\dagger V_1 = V_1 V_1^\dagger = \nu_1(1) \mathbb{1}$  and  $V_2^\dagger V_2 = V_2 V_2^\dagger = \nu_1(2) \mathbb{1}$ . Moreover, (5a) and (5b) imply that  $\nu_1(1) = 1 - \nu_1(2)$ . However, this implies that  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are not jointly linearly independent. By Corollary 1  $\rho$  is not extremal in  $\mathcal{C}(\frac{1}{2}\mathbb{1}, \frac{1}{2}\mathbb{1})$ . This is a contradiction.

Second, consider the case of nondegenerate singular values, i.e.,  $\nu_1(1) \neq \nu_2(1)$ . In this case Eqs. (5a) and (5b) imply that  $\nu_s(1) = 1 - \nu_s(2)$ ,  $|\varphi_s\rangle = |\varphi'_s\rangle$  and  $|\psi_s\rangle = |\psi'_s\rangle$  for  $s=1, 2$ . By direct computation it is easily verified that  $V_1^\dagger V_2 = V_2^\dagger V_1$  and  $V_1 V_2^\dagger = V_2 V_1^\dagger$ . This implies that  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are not jointly linearly independent. Again by Corollary 1  $\rho$  is not extremal in  $\mathcal{C}(\frac{1}{2}\mathbb{1}, \frac{1}{2}\mathbb{1})$ . A contradiction.

We summarize our results in the following proposition.

*Proposition 1: In dimension  $2 \times 2$  the extremal states in  $\mathcal{C}(\frac{1}{2}\mathbb{1}, \frac{1}{2}\mathbb{1})$  are precisely the projectors onto the subspaces spanned by maximally entangled pure wave functions.*

Proposition 1 has previously been found, using different methods, by Parthasarathy in Ref. 5.

**B. A three dimensional example**

From the preceding example it is clear that also in higher dimensions all projectors onto the subspaces spanned by maximally entangled wave functions are extremal elements in  $\mathcal{C}((1/d)\mathbb{1}, (1/d)\mathbb{1})$ . However, in the present section we show that the extension of Proposition 1 to higher dimensions does not hold. In other words the set of extremal states in  $\mathcal{C}((1/d)\mathbb{1}, (1/d)\mathbb{1})$  is not exhausted by the projectors onto maximally entangled pure states. Here we use our characterization of extremal states in  $\mathcal{C}((1/d)\mathbb{1}, (1/d)\mathbb{1})$  to construct an explicit counterexample in dimension  $3 \times 3$ .

Denote by  $\{|i\rangle\}_{i=1}^3$  the canonical real orthonormal basis of  $\mathbb{C}^3$ . Define the following operators:

$$V_1 = \frac{1}{\sqrt{2}}(|1\rangle\langle 1| + |2\rangle\langle 3|), \tag{6a}$$

$$V_2 = \frac{1}{\sqrt{2}}(|2\rangle\langle 2| + |3\rangle\langle 1|), \tag{6b}$$

$$V_3 = \frac{1}{\sqrt{2}}(|3\rangle\langle 3| + |1\rangle\langle 2|). \tag{6c}$$

By explicit calculation one checks that  $\sum_{j=1}^3 V_j^\dagger V_j = \sum_j V_j V_j^\dagger = 1$ . Moreover,

$$V_1^\dagger V_2 = V_3 V_1^\dagger = \frac{1}{2}|3\rangle\langle 2|, \tag{7a}$$

$$V_1^\dagger V_3 = V_3 V_2^\dagger = \frac{1}{2}|1\rangle\langle 2|, \tag{7b}$$

$$V_2^\dagger V_3 = V_1 V_2^\dagger = \frac{1}{2}|1\rangle\langle 3|, \tag{7c}$$

$$V_2^\dagger V_1 = V_1 V_3^\dagger = \frac{1}{2}|2\rangle\langle 3|, \tag{7d}$$

$$V_3^\dagger V_1 = V_2 V_3^\dagger = \frac{1}{2}|2\rangle\langle 1|, \tag{7e}$$

$$V_2^\dagger V_2 = V_2 V_3^\dagger = \frac{1}{2}|3\rangle\langle 1|. \tag{7f}$$

Hence  $\{V_i^\dagger V_j\}_{ij}$  and  $\{V_j V_i^\dagger\}_{ij}$  are both linearly independent and thus by Lemma 1 jointly linearly independent. By Corollary 1 the state

$$\rho := \frac{1}{3} \sum_{ijk=1}^3 V_j^\dagger |i\rangle\langle k| V_j \otimes |i\rangle\langle k| \tag{8}$$

is extremal in  $\mathcal{C}(\frac{1}{3}1, \frac{1}{3}1)$ . An explicit calculation gives the following matrix representation of  $\rho$  in the canonical product basis in lexicographic order:

$$\rho = \frac{1}{6} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{9}$$

This state is entangled but not maximally entangled and an extremal element of  $\mathcal{C}(\frac{1}{3}1, \frac{1}{3}1)$ .

**C. Higher dimensions**

It is possible to construct counterexamples to Proposition 1 also in higher dimensions. For instance, consider  $\mathbb{C}^2 \otimes \mathbb{C}^2$ . We denote the canonical basis of  $\mathbb{C}^4$  as usual by  $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$ . The three dimensional example above can be generalized to dimension  $4 \times 4$  by letting

$$V_1 = \frac{1}{\sqrt{3}}(|1\rangle\langle 1| + |2\rangle\langle 4| + |3\rangle\langle 2|),$$

$$V_2 = \frac{1}{\sqrt{3}}(|2\rangle\langle 2| + |3\rangle\langle 1| + |4\rangle\langle 3|),$$

$$V_3 = \frac{1}{\sqrt{3}}(|3\rangle\langle 3| + |4\rangle\langle 2| + |1\rangle\langle 4|),$$

$$V_4 = \frac{1}{\sqrt{3}}(|4\rangle\langle 4| + |1\rangle\langle 3| + |2\rangle\langle 1|).$$

It is straightforward to show that both  $(V_i^\dagger V_j)_{ij}$  and  $(V_j V_i^\dagger)_{ij}$  are linearly independent families. Thus an analysis similar to the one given above shows that

$$\rho := \frac{1}{4} \sum_{i,j,k=1}^4 V_j^\dagger |i\rangle\langle k| V_j \otimes |i\rangle\langle k| \quad (10)$$

is extremal in  $\mathcal{C}(\frac{1}{4}\mathbb{1}, \frac{1}{4}\mathbb{1})$  but is not a maximally entangled pure state. It is easy to construct similar counterexamples also in higher dimensions. It seems therefore likely that there are counterexamples to Proposition 1 in all dimensions greater than 2.

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