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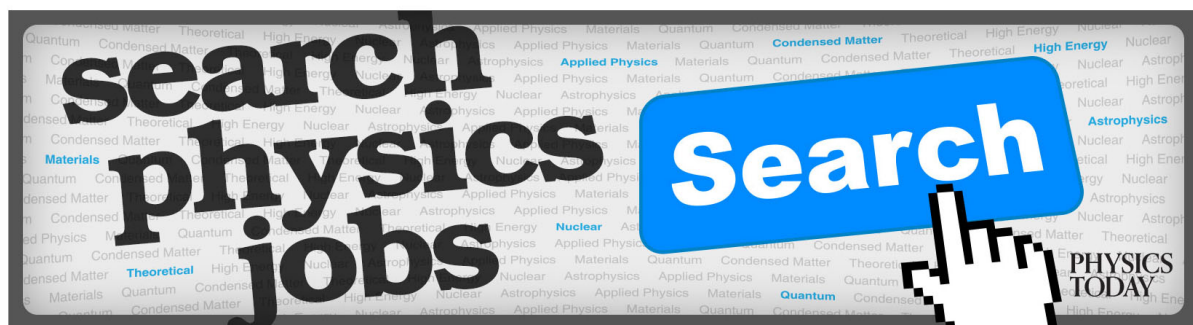
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# On the convex structure of process positive operator valued measures

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Measurements on quantum channels are described by so-called process positive operator valued measures, or process POVMs. We study implementing schemes of extremal process POVMs. As it turns out, the corresponding measurement must satisfy certain extremality property, which is stronger than the usual extremality given by the convex structure. This property motivates the introduction and investigation of the  $\mathcal{A}$ -convex structure of POVMs, which generalizes both the usual convex and  $C^*$ -convex structures. We show that extremal points and faces of the set of process POVMs are closely related to  $\mathcal{A}$ -extremal points and  $\mathcal{A}$ -faces of POVMs, for a certain subalgebra  $\mathcal{A}$ . We also give a characterization of  $\mathcal{A}$ -extremal and  $\mathcal{A}$ -pure POVMs. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4935072>]

## I. INTRODUCTION AND BASIC DEFINITIONS

Process positive operator valued measures, or process POVMs, were introduced by Ziman,<sup>22</sup> as a mathematical tool for description of measurements on quantum channels. Similar to the usual POVMs, which represent quantum observables, process POVMs are sequences of positive operators, or more generally  $\sigma$ -additive measures with values in the set of positive operators, but satisfying a different normalization condition. Independently, the same concept, called quantum 1-testers, was studied by Refs. 4 and 5, and also in Ref. 10, as measuring quantum co-strategies.

Similarly to other quantum devices, the set of all process POVMs is convex. In many cases, the convex structure determines the performance of the corresponding measurements; for example, optimal measurements with respect to convex figures of merit are given by extremal process POVMs. On the other hand, the set of process POVMs can also be the subject of statistical inference and the convex structure plays a decisive role in discrimination tasks, see Refs. 14 and 19.

Physically, any measurement on channels can be realized by applying the channel on a part of an input state  $\rho$  and consequently measuring the outcome by a usual POVM  $M$ . The aim of the present paper is to describe the extreme points and faces of the set of process POVMs in terms of these implementing schemes. It is easy to see that there is a lot of such schemes for the same process POVM, but under certain minimality conditions, the input state  $\rho$  and measurement  $M$  are unique up to a unitary conjugation. It was shown in Refs. 3 and 12 that a process POVM is extremal if and only if the POVM  $M$  in such a minimal representation is also an extremal process POVM (note that any POVM is a multiple of a process POVM, describing a channel measurement with maximally entangled input state). In the present work, we obtain a characterization within the set of POVMs, more precisely, in terms of its  $C^*$ -convex structure.

The notion of  $C^*$ -convexity of subsets of operators was introduced and studied in Refs. 15, 11, 7, and 16. Roughly speaking, instead of numbers in the interval  $(0,1)$ , the coefficients of a  $C^*$ -convex combination are operators forming a resolution of the identity. The  $C^*$ -extreme points of the set of POVMs, or more generally of the set of unital completely positive maps from a  $C^*$ -algebra into the algebra  $B(\mathcal{H})$  of bounded operators on a finite dimensional Hilbert space, were

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studied in Refs. 8 and 9. In particular, it was proved that a POVM is  $C^*$ -extremal if and only if it is projection valued. We propose a natural extension of this notion, containing both  $C^*$ -convexity and usual convexity, such that the coefficients of convex combinations are restricted to a given subalgebra  $\mathcal{A} \subseteq B(\mathcal{H})$ . We show that extremal elements and faces of the set of process POVMs correspond to  $\mathcal{A}$ -extremal elements and  $\mathcal{A}$ -faces of the representing POVMs, for some subalgebra  $\mathcal{A}$ . We also describe the face generated by a process POVM, implemented by a scheme with  $\mathcal{A}$ -extremal POVM. In particular, we show that such a process POVM is not necessarily extremal, but any element in its convex decomposition is obtained by a choice of the input state, while keeping the same measurement.

The outline of the paper is as follows. In the rest of this section, we introduce some basic notations and definitions. In Section II, we introduce the notion of  $\mathcal{A}$ -convexity and state some of its properties. All the results needed in this paper are proved similarly as in the  $C^*$ -convex case, and we give some of the proofs in Sec. V. A more general characterization of  $\mathcal{A}$ -extremal generalized states on a  $C^*$ -algebra  $\mathcal{B}$  will be given elsewhere. Process POVMs and their representing triples are discussed in Section III, and Section IV contains the main results.

Let  $\mathcal{H}$  be a Hilbert space, with  $d_{\mathcal{H}} := \dim(\mathcal{H}) < \infty$ . We denote the set of (bounded) linear operators on  $\mathcal{H}$  by  $B(\mathcal{H})$ , the set of positive operators by  $B(\mathcal{H})^+$ , and the set of density operators, that is positive operators with unit trace, by  $\mathfrak{S}(\mathcal{H})$ .

Measurements on the system are represented by POVMs. In general, these are defined on a  $\sigma$ -algebra of measurable subsets of the set  $X$  of outcomes, but we will only deal with  $X = \{1, \dots, n\}$ . In this case, a POVM is a collection of positive operators  $M_1, \dots, M_n$  on  $\mathcal{H}$ , such that  $\sum_i M_i = I$ . If the system is in some state  $\rho \in \mathfrak{S}(\mathcal{H})$ , the probability of obtaining the outcome  $i \in X$  is given by  $\text{Tr } \rho M_i$ . In this way, POVMs correspond precisely to affine maps from the state space to the probability simplex  $P_n$ . We will denote the set of  $n$ -outcome POVMs by  $\mathcal{M}(\mathcal{H}, n)$ .

*Remark 1.* Let  $\mathcal{K} \subseteq \mathcal{H}$  be a subspace and let  $P : \mathcal{H} \rightarrow \mathcal{K}$  be the corresponding projection. For any  $M \in \mathcal{M}(\mathcal{K}, n)$ , we put  $\tilde{M}_i = M_i + \frac{1}{n}(I - P)$ , then  $\tilde{M} \in \mathcal{M}(\mathcal{H}, n)$ . In this way, we may, and will, identify  $\mathcal{M}(\mathcal{K}, n)$  with a subset of  $\mathcal{M}(\mathcal{H}, n)$ .

Let  $\mathcal{L}(\mathcal{H}, \mathcal{K})$  denote the set of linear maps  $B(\mathcal{H}) \rightarrow B(\mathcal{K})$  and let  $\mathcal{C}(\mathcal{H}, \mathcal{K})$  be the set of channels, that is, completely positive trace preserving maps. The Choi isomorphism

$$C : \phi \mapsto (\phi \otimes id_{\mathcal{H}})(\psi_{\mathcal{H}}) \in B(\mathcal{K} \otimes \mathcal{H})$$

maps  $\mathcal{L}(\mathcal{H}, \mathcal{K})$  onto  $B(\mathcal{K} \otimes \mathcal{H})$  and the set of completely positive maps onto  $B(\mathcal{K} \otimes \mathcal{H})^+$ . Here,

$$\psi_{\mathcal{H}} = \sum_{i,j} |i\rangle\langle j| \otimes |i\rangle\langle j|$$

for some fixed orthonormal basis (ONB)  $\{|i\rangle\}$  in  $\mathcal{H}$  and  $id_{\mathcal{H}}$  is the identity map.

Let  $|\xi\rangle \in \mathcal{H} \otimes \mathcal{H}_0$  be a unit vector. Then, there are orthonormal bases  $|e_1\rangle, \dots, |e_{d_{\mathcal{H}}}\rangle$  and  $|f_1\rangle, \dots, |f_{d_{\mathcal{H}_0}}\rangle$  of  $\mathcal{H}$  and  $\mathcal{H}_0$ , such that

$$|\xi\rangle = \sum_{i=1}^k \alpha_i |e_i\rangle \otimes |f_i\rangle,$$

with  $\alpha_i > 0$ , this is the Schmidt decomposition of  $|\xi\rangle$ . The number  $k \leq d_{\mathcal{H}} \wedge d_{\mathcal{H}_0}$  of nonzero coefficients is called the Schmidt rank of  $|\xi\rangle$  and is denoted by  $SR(\xi)$ . Clearly,  $SR(\xi)$  is the rank of  $\text{Tr}_{\mathcal{H}} |\xi\rangle\langle\xi|$  or  $\text{Tr}_{\mathcal{H}_0} |\xi\rangle\langle\xi|$ . If  $\rho$  is a mixed state in  $\mathfrak{S}(\mathcal{H} \otimes \mathcal{H}_0)$ , then its Schmidt number  $SN(\rho)$  is the smallest  $k$  such that  $\rho$  can be expressed as a convex combination of pure states with Schmidt rank at most  $k$ , Ref. 21.

Let  $\xi_1, \dots, \xi_{d_{\mathcal{H}}} \in \mathcal{H}_0$  be such that  $|\xi\rangle = \sum_i |i\rangle \otimes |\xi_i\rangle$ . Let  $T : \mathcal{H} \rightarrow \mathcal{H}_0$  be the linear operator defined by  $T|i\rangle = |\xi_i\rangle$ , then  $\text{Tr } T^*T = 1$ ; moreover,

$$|\xi\rangle = |T\rangle\rangle := \sum_i |i\rangle \otimes T|i\rangle$$

and the map  $T \mapsto |T\rangle\rangle$  defines a linear isomorphism of the set of linear operators  $\mathcal{H} \rightarrow \mathcal{H}_0$  onto  $\mathcal{H} \otimes \mathcal{H}_0$ . We have  $SR(|T\rangle\rangle) = \text{rank}(T)$ .

## II. THE $\mathcal{A}$ -CONVEX STRUCTURE OF POVMs

In this paragraph, we introduce the notion of  $\mathcal{A}$ -convexity,  $\mathcal{A}$ -extreme points, and  $\mathcal{A}$ -faces for POVMs on  $B(\mathcal{H})$ , where  $\mathcal{A}$  is a  $C^*$ -subalgebra in  $B(\mathcal{H})$ . The results used in this paper are similar to the  $C^*$ -convex case, see Example 2 below.

Let  $\mathcal{A} \subseteq B(\mathcal{H})$  be a subalgebra and let  $M, N \in \mathcal{M}(\mathcal{H}, n)$ . We say that  $M$  and  $N$  are  $\mathcal{A}$ -equivalent, in notation  $M \sim_{\mathcal{A}} N$ , if there is a unitary  $U \in \mathcal{A}$  such that  $U^* M_i U = N_i$ , for all  $i$ . Let  $M, N^1, \dots, N^k \in \mathcal{M}(\mathcal{H}, n)$ , then  $M$  is an  $\mathcal{A}$ -convex combination of  $N^1, \dots, N^k$  if there are some elements  $X_1, \dots, X_k \in \mathcal{A}$ ,  $\sum_j X_j^* X_j = I$ , such that  $M = \sum_j X_j^* N^j X_j$ , that is,

$$M_i = \sum_j X_j^* N_i^j X_j, \quad i = 1, \dots, n. \quad (1)$$

An  $\mathcal{A}$ -convex combination is called proper if  $X_i$  is an invertible element in  $\mathcal{A}$ , for all  $i$ . It is clear that the set  $\mathcal{M}(\mathcal{H}, n)$  is  $\mathcal{A}$ -convex, in the sense that it contains all  $\mathcal{A}$ -convex combinations of its elements. A POVM  $M \in \mathcal{M}(\mathcal{H}, n)$  is  $\mathcal{A}$ -extremal if whenever  $M$  is a proper  $\mathcal{A}$ -convex combination of some POVMs  $N^1, \dots, N^k$ , then  $N^j \sim_{\mathcal{A}} M$ .

*Example 1.* Let  $\mathcal{A} = \mathbb{C}I$ , then  $\mathcal{A}$ -convexity coincides with the usual notion of convexity. In the general context of  $C^*$ -algebras, the extremal elements of the set of POVMs, regarded as (completely) positive maps from a commutative  $C^*$ -algebra into  $B(\mathcal{H})$ , were characterized in Ref. 1, see also Refs. 20, 17, and 6 for different formulations of the extremality condition. In our setting, the condition can be stated as follows: let  $P_i$  be the projection onto the support of  $M_i$ ,  $i = 1, \dots, n$ . Then,  $M$  is extremal if and only if the subspaces  $P_i \mathcal{H}$  are weakly independent, that is,  $D_i \in B(P_i \mathcal{H})$  and  $\sum_i D_i = 0$  implies  $D_i = 0$  for all  $i$  (compare this condition with Lemmas 3 and 4 below).

*Example 2.* If  $\mathcal{A} = B(\mathcal{H})$ , then  $\mathcal{A}$ -convexity is the same as  $C^*$ -convexity. In the context of  $C^*$ -algebras, this notion of convexity, along with the related extremality properties, was studied in Refs. 15, 11, 7, and 16.  $C^*$ -convexity for sets of generalized states, containing POVMs as a special case, was studied in Refs. 9 and 8. In particular, it was proved that a POVM is  $C^*$ -extremal in  $\mathcal{M}(\mathcal{H}, n)$  if and only if it is projection-valued. We give an alternative proof of this fact in Section V (Corollary 4).

We will also need the notion of an  $\mathcal{A}$ -face of  $\mathcal{M}(\mathcal{H}, n)$ . This is defined as a subset  $\mathcal{F}$  such that whenever  $\mathcal{F}$  contains a proper  $\mathcal{A}$ -convex combination of some elements  $N^1, \dots, N^k \in \mathcal{M}(\mathcal{H}, n)$ , then also  $N^j \in \mathcal{F}$  for all  $j$ , see Ref. 16 for a definition of a  $C^*$ -face of a  $C^*$ -convex set. Note that, just as in the case of a  $C^*$ -face, an  $\mathcal{A}$ -face does not have to be  $\mathcal{A}$ -convex, or even convex.

*Lemma 1.* Let  $M \in \mathcal{M}(\mathcal{H}, n)$  be  $\mathcal{A}$ -extremal then

$$\mathcal{F}_M = \{U^* M U, U \text{ is a unitary in } \mathcal{A}\}$$

is a compact  $\mathcal{A}$ -face of  $\mathcal{M}(\mathcal{H}, n)$ .

*Proof.* It is clear that  $\mathcal{F}_M$  is an  $\mathcal{A}$ -face. Compactness follows from compactness of the unitary group in  $\mathcal{A}$ .  $\square$

The proofs of the lemmas below can be found in Section V.

*Lemma 2.* Let  $\mathcal{F} \subset \mathcal{M}(\mathcal{H}, n)$  be a compact  $\mathcal{A}$ -face. Let  $M = \sum_j X_j^* N^j X_j \in \mathcal{F}$  be an  $\mathcal{A}$ -convex combination. Then for all  $j$ , there is some  $L^j \in \mathcal{M}(\mathcal{H}, n)$  such that  $Q_j N^j Q_j + Q_j^\perp L^j Q_j^\perp \in \mathcal{F}$ , where  $Q_j$  is the range projection of  $X_j$ .

We next characterize the  $\mathcal{A}$ -extremal POVMs.

*Lemma 3.* Let  $M \in \mathcal{M}(\mathcal{H}, n)$ , then  $M$  is  $\mathcal{A}$ -extremal if and only if  $0 \leq D_i \leq M_i$ ,  $i = 1, \dots, n$  and  $\sum_i D_i \in \mathcal{A}$  implies that there is some  $X \in \mathcal{A}$  such that  $D_i = X^* M_i X$ ,  $i = 1, \dots, n$ .

It is not clear in general whether for subalgebras  $\mathcal{A} \subseteq \mathcal{B}$ ,  $\mathcal{B}$ -extremality implies  $\mathcal{A}$ -extremality, but some results can be obtained for the inclusions  $\mathbb{C}I \subseteq \mathcal{A} \subseteq B(\mathcal{H})$ . One can prove exactly the same way as for the  $C^*$ -extremal case<sup>8</sup> that any  $\mathcal{A}$ -extremal POVM is extremal in the usual sense. Further, the corollary below shows that a projection valued measure is  $\mathcal{A}$ -extremal, for any  $\mathcal{A} \subseteq B(\mathcal{H})$  (see Example 2).

*Corollary 1.* Let  $P \in \mathcal{M}(\mathcal{H}, n)$  be projection-valued. Then,  $P$  is  $\mathcal{A}$ -extremal, for any subalgebra  $\mathcal{A} \subseteq B(\mathcal{H})$ .

*Proof.* Let  $0 \leq D_i \leq P_i$  be such that  $D := \sum_i D_i \in \mathcal{A}$ . Then,  $D$  commutes with all  $P_i$  and

$$D_i = DP_i = D^{1/2}P_iD^{1/2}.$$

By Lemma 3,  $P$  is  $\mathcal{A}$ -extremal. □

We say that an element  $M \in \mathcal{M}(\mathcal{H}, n)$  is  $\mathcal{A}$ -irreducible if the only projections in  $\mathcal{A}$  commuting with all  $M_1, \dots, M_n$  are 0 and  $I$ . If  $M$  is  $\mathcal{A}$ -extremal and  $\mathcal{A}$ -irreducible, then  $M$  is called  $\mathcal{A}$ -pure (cf. Ref. 8).

*Lemma 4.* Let  $M \in \mathcal{M}(\mathcal{H}, n)$  and let  $P_i$  be the support projections of  $M_i$ ,  $i = 1, \dots, n$ . Then,  $M$  is  $\mathcal{A}$ -pure if and only if  $D_i \in B(P_i\mathcal{H})$ ,  $\sum_i D_i \in \mathcal{A}$ ,  $i = 1, \dots, n$  implies that there is some  $z \in \mathbb{C}$  such that  $D_i = zM_i$ ,  $i = 1, \dots, n$ .

### III. PROCESS POVMs AND THEIR REPRESENTATIONS

A measurement on quantum channels with outcomes in the set  $X = \{1, \dots, n\}$  is naturally defined as an affine map  $\mathbf{m} : C(\mathcal{H}, \mathcal{K}) \rightarrow \mathcal{P}(X)$ , the set of probability distributions over  $X$ . For  $\Phi \in C(\mathcal{H}, \mathcal{K})$  and  $i \in X$ , the value  $\mathbf{m}(\Phi)_i$  is interpreted as the probability that the outcome of the measurement is  $i$  if the true channel is  $\Phi$ . Similarly to usual quantum measurements, there is a collection of positive operators  $F_1, \dots, F_n$  associated with  $\mathbf{m}$ ,<sup>13</sup> but acting on the tensor product  $\mathcal{K} \otimes \mathcal{H}$  and with the normalization  $\sum_i F_i = I_{\mathcal{K}} \otimes \sigma$ , for some  $\sigma \in \mathfrak{S}(\mathcal{H})$ . The relation of  $F$  and  $\mathbf{m}$  is

$$\mathbf{m}(\Phi)_i = \text{Tr } F_i C(\Phi), \quad i = 1, \dots, n.$$

Any collection  $\{F_1, \dots, F_n\}$  of positive operators with this property is called a process POVM (see Ref. 22). Moreover, it is easy to see that any process POVM defines a measurement on channels, in the above sense. We will denote the set of all process POVMs on  $\mathcal{K} \otimes \mathcal{H}$  with  $n$  outcomes by  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$ .

To save some space and simplify notations, we identify  $B(\mathcal{H})$  with the subalgebra  $I_{\mathcal{K}} \otimes B(\mathcal{H}) \subseteq B(\mathcal{K} \otimes \mathcal{H})$ . Similarly, operators  $T : \mathcal{H} \rightarrow \mathcal{H}_0$  will be identified with their natural extensions  $I_{\mathcal{K}} \otimes T : \mathcal{K} \otimes \mathcal{H} \rightarrow \mathcal{K} \otimes \mathcal{H}_0$ .

An obvious way to perform a measurement on channels is to apply the channel to an input state (possibly on the system coupled with an ancilla) and measure the outcome. The next proposition shows that indeed all measurements are obtained in this way. Moreover, it gives a certain representation result for process POVMs.

*Proposition 1 (Ref. 22).* Let  $(\mathcal{H}_0, \rho, M)$  be a triple consisting of a Hilbert space  $\mathcal{H}_0$ , a state  $\rho \in \mathfrak{S}(\mathcal{H} \otimes \mathcal{H}_0)$ , and a POVM  $M \in \mathcal{M}(\mathcal{K} \otimes \mathcal{H}, n)$ . Then, there is a unique process POVM  $F \in \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  such that

$$\text{Tr } C(\Phi)F_i = \text{Tr } M_i(\Phi \otimes id_{\mathcal{H}_0})(\rho), \quad i = 1, \dots, n, \quad \Phi \in \mathcal{L}(\mathcal{H}, \mathcal{K}). \quad (2)$$

Conversely, for any  $F \in \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$ , there exists a triple  $(\mathcal{H}_0, \rho, M)$  with a pure state  $\rho$ , such that (2) holds.

*Proof.* Let  $(\mathcal{H}_0, \rho, M)$  be such a triple. By the Choi isomorphism, there exists a completely positive map  $\Phi_\rho : B(\mathcal{H}) \rightarrow B(\mathcal{H}_0)$  such that  $(id_{\mathcal{H}} \otimes \Phi_\rho)(\psi_{\mathcal{H}}) = \rho$ . This map is given by

$$\Phi_\rho(A) = \text{Tr}_{\mathcal{H}}[\rho A^t], \quad A \in B(\mathcal{H}),$$

where  $A^t$  is the transpose of  $A$  with respect to the ONB  $\{|i\rangle\}$ . For  $\Phi \in \mathcal{L}(\mathcal{H}, \mathcal{K})$ ,

$$\mathrm{Tr} M_i(\Phi \otimes id_{\mathcal{H}_0})(\rho) = \mathrm{Tr} M_i(\Phi \otimes \Phi_\rho)(\psi_{\mathcal{H}}) = \mathrm{Tr} F_i C(\Phi),$$

with

$$F_i = (id \otimes \Phi_\rho^*)(M_i),$$

where  $\Phi_\rho^* : B(\mathcal{H}_0) \rightarrow B(\mathcal{H})$  is the adjoint of  $\Phi_\rho$  with respect to the Hilbert-Schmidt inner product, that is,

$$\Phi_\rho^*(B) = (\mathrm{Tr}_{\mathcal{H}_0}[B\rho])^t, \quad B \in B(\mathcal{H}_0). \quad (3)$$

Since  $0 \leq M_i \leq I$ ,  $\sum_i M_i = I$  and  $\Phi_\rho^*$  is completely positive, we have  $F_i \geq 0$  and  $\sum_i F_i = \sigma$ , where

$$\sigma := \Phi_\rho^*(I_{\mathcal{H}_0}) = (\mathrm{Tr}_{\mathcal{H}_0}\rho)^t \in \mathfrak{S}(\mathcal{H}).$$

Hence,  $F = \{F_1, \dots, F_n\}$  is a process POVM. Uniqueness follows from the fact that  $C$  is an isomorphism  $\mathcal{L}(\mathcal{H}, \mathcal{K})$  onto  $B(\mathcal{K} \otimes \mathcal{H})$ .

Conversely, let  $F$  be a process POVM,  $\sum_i F_i = \sigma$ ,  $\sigma \in \mathfrak{S}(\mathcal{H})$ . Let  $\mathrm{supp}(\sigma)$  be the projection onto the support of  $\sigma$  and let  $\mathcal{H}_0 = \mathrm{supp}(\sigma)\mathcal{H}$ . Then,  $\mathrm{supp}(F_i) \leq \mathrm{supp}(\sigma)$  and we may put  $M_i := \sigma^{-1/2} F_i \sigma^{-1/2} \in B(\mathcal{K} \otimes \mathcal{H}_0)$ . Clearly,  $M_i \geq 0$  and  $\sum_i M_i = I_{\mathcal{K} \otimes \mathcal{H}_0}$ , so that  $M \in \mathcal{M}(\mathcal{K} \otimes \mathcal{H}_0, n)$ . Moreover, for  $\Phi \in \mathcal{L}(\mathcal{H}, \mathcal{K})$ ,

$$\mathrm{Tr} F_i C(\Phi) = \mathrm{Tr} M_i \sigma^{1/2} C(\Phi) \sigma^{1/2} = \mathrm{Tr} M_i(\Phi \otimes id)(\rho),$$

where

$$\rho = \sigma^{1/2} \psi_H \sigma^{1/2}$$

is a pure state in  $\mathfrak{S}(\mathcal{H} \otimes \mathcal{H}_0)$ . Then,  $(\mathcal{H}_0, \rho, M)$  is the required triple with a pure input state.  $\square$

Any triple satisfying (2) will be called a representation of  $F$ . If  $(\mathcal{H}_0, \rho, M)$  and  $(\mathcal{H}'_0, \rho', M')$  are representations of the same process POVM  $F$ , we will say that the triples are equivalent and write

$$(\mathcal{H}_0, \rho, M) \simeq (\mathcal{H}'_0, \rho', M') \simeq F.$$

The proof of the following lemma is straightforward.

*Lemma 5. Let  $\rho \in \mathfrak{S}(\mathcal{H} \otimes \mathcal{H}_0)$  and  $M' \in \mathcal{M}(\mathcal{K} \otimes \mathcal{H}'_0, n)$ . Then for any  $\chi \in C(\mathcal{H}_0, \mathcal{H}'_0)$ ,*

$$(\mathcal{H}'_0, (id \otimes \chi)(\rho), M') \simeq (\mathcal{H}_0, \rho, (id \otimes \chi^*)(M')).$$

Let  $(\mathcal{H}_0, \rho, M) \simeq F$  and assume the input state  $\rho$  is pure. Then,  $\rho = |T\rangle\langle T|$  and  $\Phi_\rho^*(a) = T^* a T$  for some  $T : \mathcal{H} \rightarrow \mathcal{H}_0$ . By the proof of Lemma 1,

$$F_j = T^* M_j T, \quad j = 1, \dots, n. \quad (4)$$

We say that the representation (or the triple  $(\mathcal{H}_0, \rho, M)$ ) is minimal if the input state is pure and  $T$  is surjective. It is clear that the representation constructed in the proof of Lemma 1 is minimal.

*Lemma 6. Let  $(\mathcal{H}_0, \rho, M)$  be minimal and let  $(\mathcal{H}'_0, \rho', M') \simeq (\mathcal{H}_0, \rho, M)$ . Then, there is a channel  $\chi : B(\mathcal{H}_0) \rightarrow B(\mathcal{H}'_0)$ , such that  $(id_{\mathcal{H}} \otimes \chi)(\rho) = \rho'$  and  $M = (id_{\mathcal{H}} \otimes \chi^*)(M')$ . If  $\rho'$  is pure, then  $\chi$  is an isometric channel and if  $(\mathcal{H}'_0, \rho', M')$  is minimal, then  $\chi$  is a unitary channel.*

*Proof.* By minimality,  $\rho = |T\rangle\langle T|$  with  $T : \mathcal{H} \rightarrow \mathcal{H}_0$  surjective. Suppose first that  $\rho'$  is pure,  $\rho' = |T'\rangle\langle T'|$ . Since the two triples are representations of the same process POVM  $F$ , we must have

$$T^* T = \Phi_\rho^*(I_{\mathcal{H}_0}) = \sum_j F_j = \Phi_{\rho'}^*(I_{\mathcal{H}'_0}) = (T')^* T'.$$

By considering polar decompositions of  $T$  and  $T'$ , and using the fact that  $T$  is surjective, we obtain that there is some isometry  $U : \mathcal{H}_0 \rightarrow \mathcal{H}'_0$  such that  $T' = UT$ , so that

$$\rho' = T' \psi_{\mathcal{H}}(T')^* = U \rho U^* = (id_{\mathcal{H}} \otimes Ad_U)(\rho).$$

Similarly,

$$T^*M_iT = F_i = (T')^*M'_iT' = T^*U^*M'_iUT$$

and this implies  $M = (id_H \otimes Ad_{U^*})(M')$  by surjectivity of  $T$ . If  $(\mathcal{H}'_0, \rho', M')$  is minimal, then also  $T'$  is surjective and this implies that  $U$  is unitary.

Let now  $\rho'$  be any state and let  $\rho'_0$  be its purification, that is, there is a Hilbert space  $\mathcal{H}_1$  such that  $\rho'_0 \in \mathfrak{S}(\mathcal{H} \otimes \mathcal{H}'_0 \otimes \mathcal{H}_1)$  is a pure state and  $\text{Tr}_{\mathcal{H}_1}\rho'_0 = \rho'$ . By Lemma 5, we obtain

$$(\mathcal{H}_0, \rho, M) \simeq (\mathcal{H}'_0, \rho', M') = (\mathcal{H}'_0, \text{Tr}_{\mathcal{H}_1}(\rho'_0), M') \simeq (\mathcal{H}'_0 \otimes \mathcal{H}_1, \rho'_0, M').$$

By the first part of the proof, there is some isometry  $U : \mathcal{H}_0 \rightarrow \mathcal{H}'_0 \otimes \mathcal{H}_1$  such that  $\rho'_0 = U\rho U^*$  and  $U^*M'U = M$ . Put  $\chi = \text{Tr}_{\mathcal{H}_1} \circ Ad_U$ , then  $\chi$  is a channel  $B(\mathcal{H}_0) \rightarrow B(\mathcal{H}'_0)$  and we have  $\rho' = \text{Tr}_{\mathcal{H}_1}\rho'_0 = (id_{\mathcal{H}} \otimes \chi)(\rho)$ ,  $M = (id_{\mathcal{H}} \otimes \chi^*)(M')$ .  $\square$

Let  $F$  be a process POVM and let  $\sum_j F_j = \sigma \in \mathfrak{S}(\mathcal{H})$ . Then,  $r(F) := \text{rank}(\sigma)$  will be called the rank of  $F$ .

*Lemma 7.* *Let  $F$  be a process POVM with rank  $r$ . Then, for any representation  $(\mathcal{H}_0, \rho, M) \simeq F$ , the Schmidt number of the input state  $SN(\rho) \leq r$ . If  $\rho$  is pure, then  $SN(\rho) = r$  and the representation is minimal if and only if  $\dim(\mathcal{H}_0) = r$ .*

*Proof.* By the proof of Lemma 1, there is a minimal representation  $(\mathcal{H}_0, \rho, M) \simeq F$ , where  $\mathcal{H}_0$  is the range of  $\sigma$ ; hence,  $SN(\rho) = \dim(\mathcal{H}_0) = r(F)$ . The rest follows by Lemma 6.  $\square$

*Remark 2.* If the input state is pure, we will often abuse the notation and write the triple as  $(\mathcal{H}_0, T, M)$ , instead of  $(\mathcal{H}_0, |T\rangle\langle T|, M)$ . Let  $(\mathcal{H}_0, T, M) \simeq F$  and let  $\mathcal{H}_T \subseteq \mathcal{H}_0$  be the range of  $T$ , with  $P_T$  the projection onto  $\mathcal{H}_T$  (we will keep this notation throughout the paper). Then, it is easy to see that  $(\mathcal{H}_T, T, P_T M P_T)$  is an equivalent minimal representation. On the other hand, if  $\mathcal{H}_0 \subseteq \mathcal{H}'_0$ , then  $F \simeq (\mathcal{H}'_0, T, \tilde{M})$ , where  $\tilde{M}$  is the extension of  $M$  in  $\mathcal{M}(\mathcal{K} \otimes \mathcal{H}'_0, n)$  as in Remark 1.

#### IV. EXTREME POINTS AND FACES OF $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$

It is easy to see that the set of process POVMs is convex and compact. We will now examine the extremal points and faces of the set  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  and obtain a description in terms of the minimal representing triples. As it turns out, the convex structure of  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  is closely related to the  $B(\mathcal{H}_0)$ -convex structure of  $\mathcal{M}(\mathcal{K} \otimes \mathcal{H}_0, n)$ , where  $B(\mathcal{H}_0)$  is seen as a subalgebra of  $B(\mathcal{K} \otimes \mathcal{H}_0)$ .

##### A. Extremal process POVMs

We first look at representing triples of convex combinations of process POVMs. Let  $F^1, \dots, F^m$  be process POVMs and let  $(\mathcal{H}_i, T_i, M^i) \simeq F^i$  be representations (not necessarily minimal) with pure input states. Consider a convex combination  $F = \sum \lambda_i F^i$ , with  $\lambda_i > 0$  for all  $i$ . Put

$$S := \left( \sum_i \lambda_i T_i^* T_i \right)^{1/2} \quad (5)$$

and define the maps  $X_i : \mathcal{H}_S \rightarrow \mathcal{H}_i$  by

$$X_i \xi = \lambda_i^{1/2} T_i S^{-1} \xi, \quad \xi \in \mathcal{H}_S, \quad (6)$$

where  $S^{-1}$  is the inverse of  $S$  on  $\mathcal{H}_S$  and 0 on the complement. Let also

$$N = \sum_i X_i^* M^i X_i. \quad (7)$$

Since  $\sum_i X_i^* X_i = I_{\mathcal{H}_S}$ ,  $N$  is a POVM on  $\mathcal{K} \otimes \mathcal{H}_S$  and we have

$$S^* N S = \sum_i \lambda_i T_i^* M^i T_i = \sum_i \lambda_i F^i = F.$$



Hence,  $F \simeq (\mathcal{H}_S, S, N)$  and this representation is minimal. On the other hand, let  $F$  be a process POVM and let  $F \simeq (\mathcal{H}_0, T, M)$  be a representation, with a pure input state but again minimality is not assumed. Suppose that  $M = \sum_{i=1}^m X_i^* M^i X_i$  is a  $B(\mathcal{H}_0)$ -convex combination of some  $M^i \in \mathcal{M}(\mathcal{K} \otimes \mathcal{H}_0, n)$ . Put

$$\mathcal{I} := \{i \in \{1, \dots, m\}, X_i T \neq 0\} \quad (8)$$

and for  $i \in \mathcal{I}$ , we define

$$\mu_i := \text{Tr } T^* X_i^* X_i T, \quad T_i := \mu_i^{-1/2} X_i T, \quad F^i \simeq (\mathcal{H}_0, T_i, M^i). \quad (9)$$

Then, it is easy to see that  $\mu_i > 0$ ,  $\sum_i \mu_i = 1$ ,  $F^i$  are process POVMs, and

$$F = T^* M T = \sum_i T^* X_i^* M^i X_i T = \sum_{i \in \mathcal{I}} \mu_i T_i^* M^i T_i = \sum_{i \in \mathcal{I}} \mu_i F^i.$$

Our first main result is the following characterization of minimal representations of extremal process POVMs.

**Theorem 1.** *Let  $F \in \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  and let  $(\mathcal{H}_0, T, M) \simeq F$  be a minimal representation. Then, the following statements are equivalent:*

- (i)  $F$  is extremal;
- (ii)  $M$  is  $B(\mathcal{H}_0)$ -extremal and for any representation  $(\mathcal{H}'_0, \rho', M') \simeq F$ , we have  $SN(\rho') = r(F)$ ;
- (iii)  $M$  is  $B(\mathcal{H}_0)$ -pure.

*Proof.* Suppose (i) and let  $(\mathcal{H}'_0, \rho', M') \simeq F$ . By Lemma 7,  $SN(\rho') \leq r(F)$ , with equality if  $\rho'$  is pure. Let  $\rho' = \sum_i \lambda_i \rho_i$  for some  $0 < \lambda_i < 1$ ,  $\sum_i \lambda_i = 1$  and pure states  $\rho_i$ , and assume that  $SR(\rho_k) < r(F)$  for some  $k$ . Then since  $\rho_k$  is pure,  $(\mathcal{H}'_0, \rho_k, M')$  cannot be a representation of  $F$ . Let  $F^i$  be process POVMs such that  $(\mathcal{H}'_0, \rho_i, M') \simeq F^i$ , then  $F^k \neq F$ . But then  $F = \sum_i \lambda_i F^i$ , with  $F^k \neq F$ , a contradiction. Hence, we must have  $SN(\rho') = SR(\rho_k) = r(F)$ , for all  $k$ .

Further, suppose  $M = \sum_i X_i^* M^i X_i$  is a proper  $B(\mathcal{H}_0)$ -convex combination of some  $M^i \in \mathcal{M}(\mathcal{K} \otimes \mathcal{H}_0, n)$ . Note that then  $X_i T \neq 0$  for all  $i$  and  $F = \sum_i \mu_i F^i$ , where  $F^i \simeq (\mathcal{H}_0, T_i, M^i)$  are as in (9). Since  $X_i$  is invertible and  $T$  is surjective, these are minimal representations of  $F^i$ . By extremality, we must have  $F^i = F$ , so that  $(\mathcal{H}_0, T_i, M^i) \simeq F$  for all  $i$  and by Lemma 6, this implies that  $M^i \sim_{B(\mathcal{H}_0)} M$ . Hence,  $M$  is  $B(\mathcal{H}_0)$ -extremal, this proves (ii).

Suppose (ii). We have to show that  $M$  is  $B(\mathcal{H}_0)$ -irreducible. So let  $P \in B(\mathcal{H}_0)$  be a projection such that  $PM_j = M_j P$  for all  $j$ . Let  $\chi_P : B(\mathcal{H}_0) \rightarrow B(\mathcal{H}_0)$ ,  $A \mapsto PAP + P^\perp A P^\perp$ , then  $\chi_P$  is a unital channel such that  $\chi_P^* = \chi_P$  and  $(id \otimes \chi_P)(M) = M$ . By Lemma 5,  $F \simeq (\mathcal{H}_0, (id \otimes \chi_P)(|T\rangle\langle T|), M)$  and it is clear that  $SN((id \otimes \chi_P)(|T\rangle\langle T|)) = r(F) = \text{rank}(T)$  if and only if  $P = 0$  or  $I$ . This proves (iii).

Finally, suppose (iii) and let  $F = \sum_i \lambda_i F^i$ , where  $F^i \in \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  have minimal representations  $F^i \simeq (\mathcal{H}_i, T_i, M^i)$ . Then,  $F$  has a minimal representation  $(\mathcal{H}_S, S, N)$  given by Equations (5)-(7). Clearly, we may assume that  $\mathcal{H}_i \subseteq \mathcal{H}_S$ , so that  $X_i \in B(\mathcal{H}_S)$  and  $N = \sum_i X_i^* \tilde{M}^i X_i$  is a  $B(\mathcal{H}_S)$ -convex combination of the extensions  $\tilde{M}^i \in \mathcal{M}(\mathcal{K} \otimes \mathcal{H}_S, n)$ . By Lemma 6,  $N = U^* M U$  for some unitary  $U : \mathcal{H}_0 \rightarrow \mathcal{H}_S$ , so that  $N$  is  $B(\mathcal{H}_S)$ -pure. For all  $i$  and  $j$ , we have  $D_j^i := X_i^* \tilde{M}^i X_i \leq N_j$  and  $\sum_j D_j^i = X_i^* X_i \in B(\mathcal{H}_S)$ . Lemma 4 now implies that  $D_j^i = s_i N_j$  for all  $j$  and some  $s_i \in [0, 1]$ . But then we must have

$$F^i = T_i^* M^i T_i = S^* N S = F, \quad \forall i$$

and  $F$  is extremal. □

## B. Faces of $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$

Let  $\mathcal{H}_0 \subseteq \mathcal{H}$  be a subspace. Then, any  $F \in \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  with  $r(F) \leq \dim(\mathcal{H}_0) =: r$  has a representation with ancilla  $\mathcal{H}_0$  and a pure input state. Once the ancilla is fixed, any such  $F$  can be represented by a pair  $(T, M)$ , where

$$T \in \mathcal{T} := \{T : \mathcal{H} \rightarrow \mathcal{H}_0, \text{Tr } T^* T = 1\}$$



and  $M \in \mathcal{M} := \mathcal{M}(\mathcal{K} \otimes \mathcal{H}_0, n)$ . Conversely, for any  $(T, M) \in \mathcal{T} \times \mathcal{M}$ ,  $(\mathcal{H}_0, T, M) \simeq F$  with  $r(F) \leq r$ . Equivalence of representations defines an equivalence relation on  $\mathcal{T} \times \mathcal{M}$  as  $(T, M) \simeq (T', M')$  if and only if  $T^*MT = (T')^*M'T'$ . Note that  $(T, M) \simeq (T', M')$  if and only if there is a unitary  $U \in B(\mathcal{H}_0)$  such that

$$T' = UT \text{ and } P_T M P_T = P_T U^* M' U P_T. \quad (10)$$

Let  $\mathcal{F} \subseteq \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  and let  $r := \sup_{F \in \mathcal{F}} r(F)$ . Fix a subspace  $\mathcal{H}_0 \subseteq \mathcal{H}$  with  $\dim(\mathcal{H}_0) = r$  and let  $\mathcal{T}$  and  $\mathcal{M}$  be as above. Let  $S_{\mathcal{F}} = \{(T, M) \in \mathcal{T} \times \mathcal{M}, T^*MT \in \mathcal{F}\}$  and let  $\mathcal{M}_{\mathcal{F}}$  and  $\mathcal{T}_{\mathcal{F}}$  be the projections of  $S_{\mathcal{F}}$  in  $\mathcal{M}$  and  $\mathcal{T}$ . We also denote by  $\mathcal{H}_{\mathcal{F}}$  the subspace in  $\mathcal{H}$  generated by the ranges of  $T^*$  for  $T \in \mathcal{T}_{\mathcal{F}}$ .

Note that if  $\mathcal{F}$  is closed, then  $S_{\mathcal{F}}$ ,  $\mathcal{M}_{\mathcal{F}}$ , and  $\mathcal{T}_{\mathcal{F}}$  are compact. Indeed, since both  $\mathcal{M}$  and  $\mathcal{T}$  are compact sets, so is the product  $\mathcal{T} \times \mathcal{M}$ . The map  $(T, M) \mapsto T^*MT$  is continuous and  $S_{\mathcal{F}}$  is the pre-image of  $\mathcal{F}$ , so that  $S_{\mathcal{F}}$  is a closed subset of  $\mathcal{T} \times \mathcal{M}$ . It follows that  $S_{\mathcal{F}}$  is compact and so are the projections  $\mathcal{M}_{\mathcal{F}}$  and  $\mathcal{T}_{\mathcal{F}}$ .

**Theorem 2.** *Let  $\mathcal{F} \subseteq \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  and let  $\sup_{F \in \mathcal{F}} r(F) = r$ . Then,  $\mathcal{F}$  is a face of  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  if and only if the following conditions hold:*

- (i)  $\dim(\mathcal{H}_{\mathcal{F}}) = r$ ;
- (ii)  $\mathcal{M}_{\mathcal{F}}$  is a  $B(\mathcal{H}_0)$ -face of  $\mathcal{M}$ ;
- (iii) *let  $M^1, \dots, M^m \in \mathcal{M}_{\mathcal{F}}$ ,  $X_1, \dots, X_m \in B(\mathcal{H}_0)$  be such that  $\sum_i X_i^* X_i = I$  and  $T \in \mathcal{T}$ . Then,  $(T, \sum_i X_i^* M^i X_i) \in S_{\mathcal{F}}$  if and only if  $(\mu_{X_i}^{-1/2} X_i T, M^i) \in S_{\mathcal{F}}$  for all  $i$  such that  $\mu_{X_i} := \text{Tr } T^* X_i^* X_i T \neq 0$ .*

*Remark 3.* Recall that a  $B(\mathcal{H}_0)$ -face is not necessarily  $B(\mathcal{H}_0)$ -convex. Condition (iii) in the above theorem specifies those  $B(\mathcal{H}_0)$ -convex combinations of its elements that  $\mathcal{M}_{\mathcal{F}}$  contains. In particular, it implies that  $\mathcal{M}_{\mathcal{F}}$  is convex.

*Proof.* Suppose  $\mathcal{F}$  is a face. Condition (i) is a consequence of convexity of  $\mathcal{F}$ . Indeed, let  $F$  be a point in the relative interior of  $\mathcal{F}$  and let  $(T, M)$  be a corresponding pair, then  $\sum_j F_j = T^*T =: \sigma \in \mathfrak{S}(\mathcal{H})$ . Let  $T'$  be any element in  $\mathcal{T}_{\mathcal{F}}$ . Then, there is some  $M'$  such that  $(\mathcal{H}_0, T', M') \simeq F' \in \mathcal{F}$  and  $(1+s)F - sF' \in \mathcal{F}$  for some  $s > 0$ . This implies  $(1+s)\sigma - s\sigma' \in \mathfrak{S}(\mathcal{H})$ , where  $\sigma' = (T')^*T'$ . Consequently, the support of  $\sigma'$ , which is the same as the range of  $(T')^*$ , is contained in the support of  $\sigma$ . It follows that the support of  $\sigma$  is equal to  $\mathcal{H}_{\mathcal{F}}$  and (i) holds.

To prove (ii), let  $M = \sum_i X_i^* M^i X_i \in \mathcal{M}_{\mathcal{F}}$  be a proper  $B(\mathcal{H}_0)$ -convex combination of  $M^i \in \mathcal{M}$ . Then, there is some  $T \in \mathcal{T}$  such that  $(\mathcal{H}_0, T, M) \simeq F \in \mathcal{F}$  and  $F = \sum_{i \in I} \mu_i F^i$ , where  $I$  and  $F^i \simeq (\mathcal{H}_0, T_i, M^i)$  are as in (8) and (9). Since  $\mathcal{F}$  is a face,  $F^i \in \mathcal{F}$  and hence  $M^i \in \mathcal{M}_{\mathcal{F}}$  (note that all  $i$  are in  $I$  since  $X_i$  is invertible). It follows that  $\mathcal{M}_{\mathcal{F}}$  is a  $B(\mathcal{H}_0)$ -face of  $\mathcal{M}$ .

For (iii), let  $\sum_i X_i^* M^i X_i = M$  and let  $T \in \mathcal{T}$  be such that  $(\mu_{X_i}^{-1/2} X_i T, M^i) \in S_{\mathcal{F}}$  for  $\mu_{X_i} \neq 0$ . Let  $F^i \simeq (\mathcal{H}_0, \mu_{X_i}^{-1/2} X_i T, M^i)$ , then  $F^i \in \mathcal{F}$ . Since  $\mathcal{F}$  is convex and  $\sum_i \mu_{X_i} = \sum_i \text{Tr } T^* T = 1$ , we have  $F = \sum_i \mu_{X_i} F^i \in \mathcal{F}$ , so that  $(T, M) \in S_{\mathcal{F}}$ . For the converse of (iii), let  $T \in \mathcal{T}$  be such that  $T^*MT = F \in \mathcal{F}$ . Then,  $F = \sum_{i \in I} \mu_{X_i} F^i$  as in (9). Since  $\mathcal{F}$  is a face, this implies  $F^i \in \mathcal{F}$  and  $(\mu_{X_i}^{-1/2} X_i T, M^i) \in S_{\mathcal{F}}$  for all  $i \in I$ .

Conversely, assume (i)-(iii) hold. Let  $F^1, F^2 \in \mathcal{F}$ ,  $(\mathcal{H}_0, T_i, M^i) \simeq F^i$  and let  $\lambda F^1 + (1-\lambda)F^2 = F$  for some  $\lambda \in (0, 1)$ . Then,  $F \simeq (H_S, S, N)$ , where  $N = \sum_i X_i^* M^i X_i$  as in (5)-(7). We have  $H_S \subseteq H_{\mathcal{F}}$  and by (i), there is a unitary  $U : H_{\mathcal{F}} \rightarrow H_0$ . Put  $T := US \in \mathcal{T}$  and

$$Y_i := X_i U^*, \quad i = 1, 2, \quad Y_3 = I_{H_0} - P_T$$

then  $Y_i \in B(H_0)$ ,  $\sum_i Y_i^* Y_i = I$  and

$$\lambda^{-1/2} Y_1 T = T_1, \quad (1-\lambda)^{-1/2} Y_2 T = T_2, \quad Y_3 T = 0.$$

Put  $M = \sum_i Y_i^* M^i Y_i$ , where  $M^3$  is any element in  $\mathcal{M}_{\mathcal{F}}$ , then it follows by (iii) that  $(T, M) \in S_{\mathcal{F}}$ . Since clearly  $T^*MT = S^*NS$ , we have that  $F \simeq (H_S, S, N) \simeq (H_0, T, M)$  is in  $\mathcal{F}$ , so that  $\mathcal{F}$  is convex.

To prove that  $\mathcal{F}$  is a face, let  $F^1, F^2 \in \mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  and  $\lambda \in (0, 1)$  be such that  $\lambda F^1 + (1-\lambda)F^2 = F \in \mathcal{F}$ . It is clear that then  $r(F^i) \leq r(F) \leq r$ , so that there are some  $(T_i, M^i) \in \mathcal{T} \times \mathcal{M}$

such that  $(\mathcal{H}_0, T_i, M^i) \simeq F^i$ . Then,  $F$  has a minimal representation  $(\mathcal{H}_S, S, N)$  as in (5)-(7) and since  $F \in \mathcal{F}$ ,  $F \simeq (\mathcal{H}_0, T, M)$  for some  $(T, M) \in S_{\mathcal{F}}$ . By Lemma 6, there is an isometry  $V : \mathcal{H}_S \rightarrow \mathcal{H}_0$  such that  $T = VS$  and  $N = V^*MV$ . Exactly as before, we put  $Y_i = X_iV^*$  for  $i = 1, 2$  and  $Y_3 = I - P_T$ . Then,  $Y_1, Y_2, Y_3 \in B(\mathcal{H}_0)$ ,  $\sum_i Y_i^*Y_i = I_{\mathcal{H}_0}$ , and

$$M' := \sum_{i=1}^3 Y_i^* M^i Y_i,$$

with arbitrary  $M^3 \in \mathcal{M}_{\mathcal{F}}$  satisfies  $T^*M'T = S^*NS = F$ ; hence,  $(T, M') \in S_{\mathcal{F}}$ . By (ii) and Lemmas 11 and 2, there are elements  $R^i \in \mathcal{M}$ ,  $i = 1, 2$  such that

$$N^i := Q_i M^i Q_i + Q_i^\perp R^i Q_i^\perp \in \mathcal{M}_{\mathcal{F}},$$

where  $Q_i$  is the range projection of  $Y_i$ . Then, with  $N^3 = M^3$ , we have

$$M' = \sum_{i=1}^3 Y_i^* N^i Y_i.$$

By (iii),  $(\mu_{Y_i}^{-1/2} Y_i T, N^i) \in S_{\mathcal{F}}$ , with

$$\mu_{Y_i} = \text{Tr } T^* Y_i^* Y_i T = \text{Tr } S^* X_i^* X_i S = \lambda_i \text{Tr } T_i^* T_i = \lambda_i,$$

where  $\lambda_1 = \lambda$ ,  $\lambda_2 = 1 - \lambda$ . Moreover,

$$\lambda_i^{-1} T^* Y_i^* N^i Y_i T = \lambda_i^{-1} T^* Y_i^* M^i Y_i T = \lambda_i^{-1} S X_i^* M^i X_i S = T_i^* M^i T_i = F^i.$$

It follows that  $F^i \in \mathcal{F}$ ; hence,  $\mathcal{F}$  is a face of  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$ . □

### C. The face generated by a process POVM with $B(\mathcal{H}_0)$ -extremal measurement

Let  $M$  be a  $B(\mathcal{H}_0)$ -extremal element in  $\mathcal{M}$  and let  $T \in \mathcal{T}$  be surjective. Then,  $(\mathcal{H}_0, T, M)$  is a minimal representation of some process POVM  $F = T^*MT$ . As an illustration of our results, we will describe the face of  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$ , generated by  $F$ .

Let  $M$  be any element of  $\mathcal{M}(\mathcal{H}, n)$ . A Naimark representation of  $M$  is a triple  $(\tilde{\mathcal{H}}, E, J)$ , where  $\tilde{\mathcal{H}}$  is some Hilbert space,  $E \in \mathcal{M}(\tilde{\mathcal{H}}, n)$  is projection valued, and  $J : \mathcal{H} \rightarrow \tilde{\mathcal{H}}$  is an isometry such that  $M = J^*EJ$ . If moreover the set  $\{E_k J\xi, k = 1, \dots, n, \xi \in \mathcal{H}\}$  spans  $\tilde{\mathcal{H}}$ , such a representation is called minimal. In fact,  $(c_1, \dots, c_n) \mapsto \sum_j c_j M_j$  defines a completely positive map  $\mathbb{C}^n \rightarrow B(\mathcal{H})$  and  $(\tilde{\mathcal{H}}, E, J)$  is a (minimal) Stinespring representation of this map, see, for example, Ref. 18. We will denote by  $\{E\}'$  the commutant of  $\{E_1, \dots, E_n\}$  in  $B(\tilde{\mathcal{H}})$ .

**Lemma 8.** *Let  $M \in \mathcal{M}(\mathcal{H}, n)$ , with minimal Naimark representation  $M = J^*EJ$ , and let  $X \in B(\mathcal{H})$ . Then  $X^*MX \leq M$  if and only if there is some  $C \in \{E\}'$ ,  $\|C\| \leq 1$ , such that  $CJ = JX$ .*

*Proof.* Note that  $\Phi_X : (c_1, \dots, c_n) \mapsto \sum_j c_j X^* M_j X$  defines a completely positive map  $\mathbb{C}^n \rightarrow B(\mathcal{H})$  with a Stinespring representation  $(\tilde{\mathcal{H}}, E, JX)$  and the condition  $X^*MX \leq M$  is equivalent to a natural ordering of the corresponding maps. By the Radon-Nikodym theorem for completely positive maps (Ref. 1, Theorem 1.4.2.), there is some element  $0 \leq B \leq I$  in  $\{E\}'$ , such that

$$X^* M_j X = J^* E_j B J = J^* B_j J,$$

where  $B_j = E_j B$ . Let  $Q_j$  denote the support projection of  $B_j$ , then  $Q = \{Q_1, \dots, Q_n\}$  is a projection valued measure on the range  $\tilde{\mathcal{H}}_B$  of  $B$ . It follows that  $(\tilde{\mathcal{H}}_B, Q, B^{1/2}J)$  is another Stinespring representation of  $\Phi_X$ , which is obviously minimal. It follows that there is a partial isometry  $W \in B(\tilde{\mathcal{H}})$  with initial space  $\tilde{\mathcal{H}}_B$ , such that  $W B^{1/2} J = JX$  and  $W^* E_j W = Q_j \leq E_j$  for all  $j$ . This implies that  $W \in \{E\}'$ . Put  $C := W B^{1/2}$ , then  $C \in \{E\}'$ ,  $\|C\| \leq 1$  and  $CJ = JX$ . Conversely, if  $JX = CJ$ , for  $C$  as above, then for all  $j$ ,

$$X^* M_j X = X^* J^* E_j J X = J^* C^* E_j C J = J^* C^* C E_j J \leq J^* E_j J = M_j.$$

□

For  $M \in \mathcal{M}$ , we will denote  $\mathcal{L}_M := \{X \in B(\mathcal{H}_0), X^*MX \leq M\}$ . It is easy to see by Lemma 8 that  $\mathcal{L}_M$  is a compact convex subset of  $B(\mathcal{H}_0)$ , closed under multiplication but not necessarily under taking adjoints. If  $M$  is  $B(\mathcal{H}_0)$ -extremal in  $\mathcal{M}$  and  $X \in \mathcal{L}_M$ , then  $0 \leq M_j - X^*M_jX \leq M_j$  for all  $j$ , so that by Lemma 3, there is some  $Y \in B(\mathcal{H}_0)$  such that  $M_j - X^*M_jX = Y^*M_jY$ ,  $\forall j$ . It is clear that  $X^*MX + Y^*MY = M$ ,  $X^*X + Y^*Y = I$ , and  $Y \in \mathcal{L}_M$ .

Let now  $M \in \mathcal{M}$  be  $B(\mathcal{H}_0)$ -extremal and  $T \in \mathcal{T}$  surjective. Let

$$\mathcal{F}_{T,M} := \{\mu_X^{-1}T^*X^*MXT, X \in \mathcal{L}_M, \mu_X := (\text{Tr}T^*X^*XT) \neq 0\}.$$

In the rest of this section, we will prove that  $\mathcal{F}_{T,M}$  is the smallest face of  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  containing  $F = T^*MT$ . We will first find the projection  $\mathcal{M}_{T,M} := \mathcal{M}_{\mathcal{F}_{T,M}}$  of  $\mathcal{F}_{T,M}$  in  $\mathcal{M}$ .

*Lemma 9.*  $\mathcal{M}_{T,M}$  is the set of all  $N \in \mathcal{M}$ , such that there exists a projection  $Q \in B(\mathcal{H}_0)$  and a unitary  $U \in B(\mathcal{H}_0)$ , satisfying

$$QU^*NUQ = QM = MQ.$$

*Proof.* Assume  $N \in \mathcal{M}_{T,M}$ , then there is some  $S \in \mathcal{T}$  and  $X \in \mathcal{L}_M$  such that  $(S, N) \simeq (\mu_X^{-1/2}XT, M)$ . Hence, by (10), there is a unitary  $V \in B(\mathcal{H}_0)$  such that  $S = \mu_X^{-1/2}VXT$  and  $P_XMP_X = P_XV^*NVP_X$ , note that since  $T$  is surjective  $P_X = P_{XT}$ . Let  $Y \in \mathcal{L}_M$  be such that  $X^*MX + Y^*MY = M$ . This is a  $B(\mathcal{H}_0)$ -convex combination, so by Lemmas 1 and 2, we obtain that

$$W^*MW = P_XMP_X + P_X^\perp RP_X^\perp,$$

for some unitary  $W \in B(\mathcal{H}_0)$  and some  $R \in \mathcal{M}$ . Put  $Q := WP_XW^*$ ,  $U := VW^*$ , and  $R' = WRW^*$ . Then, we have

$$M = QU^*NUQ + Q^\perp R'Q^\perp,$$

so that  $QU^*NUQ = QM = MQ$ .

Conversely, let  $N$ ,  $Q$ , and  $U$  be as in the lemma, then clearly  $Q \in \mathcal{L}_M$  and  $(\mu_Q^{-1/2}QT, M) \simeq (\mu_Q^{-1/2}UQT, N)$  defines an element in  $\mathcal{F}_{T,M}$ , so that  $N \in \mathcal{M}_{T,M}$ .  $\square$

*Lemma 10.*  $\mathcal{M}_{T,M}$  is a  $B(\mathcal{H}_0)$ -face of  $\mathcal{M}$ .

*Proof.* Let  $\sum_i X_i^*M^iX_i = N \in \mathcal{M}_{T,M}$  be a proper  $B(\mathcal{H}_0)$ -convex combination of  $M^i \in \mathcal{M}$ . Let  $Q$  and  $U$  be as in Lemma 9. Then,  $\sum_i QU^*X_i^*M^iX_iUQ = QM$ , so that

$$M = \sum_i Y_i^*M^iY_i + Q^\perp MQ^\perp,$$

with  $Y_i = X_iUQ$ . By Lemmas 1 and 2, for each  $i$ , there is some  $R^i \in \mathcal{M}$  and a unitary  $W_i \in B(\mathcal{H}_0)$  such that

$$W_i^*MW_i = P_{Y_i}M^iP_{Y_i} + P_{Y_i}^\perp R^iP_{Y_i}^\perp.$$

Put  $Q_i = W_iP_{Y_i}W_i^*$ , then

$$Q_iW_iM^iW_i^*Q_i = Q_iM = MQ_i,$$

so that  $M^i \in \mathcal{M}_{T,M}$ .  $\square$

*Proposition 2.*  $\mathcal{F}_{T,M}$  is the smallest face of  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  containing  $F = T^*MT$ .

*Proof.* Let  $\mathcal{F}$  be any face containing  $F$ . Let  $X \in \mathcal{L}_M$  be such that  $\mu_X \neq 0$  and let  $Y \in \mathcal{L}_M$  be such that  $M = X^*MX + Y^*MY$ . By Theorem 2 (iii), we must have  $(\mu_X^{-1/2}XT, M) \in S_{\mathcal{F}}$ , so that  $\mathcal{F}_{T,M} \subseteq \mathcal{F}$ . It is now enough to prove that  $\mathcal{F}_{T,M}$  satisfies conditions (i) and (iii) from Theorem 2.

For (i), note that  $r = \sup_{F' \in \mathcal{F}_{T,M}} r(F') = \dim(\mathcal{H}_0)$  and if  $(S, N) \in S_{\mathcal{F}_{T,M}}$ , then  $S = \mu_X^{-1/2}UXT$  for some unitary  $U \in B(\mathcal{H}_0)$  and hence  $S^*\mathcal{H}_0 = T^*X^*U^*\mathcal{H}_0 \subseteq T^*\mathcal{H}_0$ , so that  $\mathcal{H}_{\mathcal{F}_{T,M}} \subseteq T^*\mathcal{H}_0 \subseteq \mathcal{H}_{\mathcal{F}_{T,M}}$ .

To prove (iii), let  $M^1, \dots, M^m \in \mathcal{M}$ ,  $X_1, \dots, X_m \in B(\mathcal{H}_0)$ ,  $\sum_i X_i^* X_i = I$ , and let  $S \in \mathcal{T}$ . Put  $N = \sum_i X_i^* M^i X_i$  and assume that  $(S, N) \in S_{\mathcal{F}_{M,T}}$ . As in the proof of Lemma 9, there is some  $X \in \mathcal{L}_M$ , a unitary  $V \in B(\mathcal{H}_0)$  and some  $M' \sim_{B(\mathcal{H}_0)} M$  such that  $S = \mu_X^{-1/2} V X T$  and

$$P_X V^* N V P_X = P_X M P_X = P_X M' = M' P_X.$$

Substituting for  $N$  and putting  $Y_i := X_i V P_X$ , we obtain

$$\sum_i Y_i^* M^i Y_i + P_X^\perp M' P_X^\perp = M'.$$

By Lemmas 1 and 2, for each  $i$ , there is some  $R^i \in \mathcal{M}$  and a unitary  $Z_i \in B(\mathcal{H}_0)$  such that

$$P_{Y_i} M^i P_{Y_i} + P_{Y_i}^\perp R^i P_{Y_i}^\perp = Z_i^* M Z_i.$$

It follows that

$$P_{Y_i} M^i P_{Y_i} = P_{Y_i} Z_i^* M Z_i P_{Y_i}. \quad (11)$$

Now note that  $X_i S = \mu_X^{-1/2} X_i V X T = \mu_X^{-1/2} Y_i X T$  and  $P_{X_i S} = P_{Y_i}$ . If  $\mu_i = \text{Tr } S^* X_i^* X_i S \neq 0$ , then by (10) and (11),

$$(\mu_i^{-1/2} X_i S, M^i) = (\mu_{Y_i X}^{-1/2} Y_i X T, M^i) \simeq (\mu_{Y_i X}^{-1/2} Z_i Y_i X T, M)$$

and we have

$$\begin{aligned} X^* Y_i^* Z_i^* M Z_i Y_i X &= X^* Y_i^* M^i Y_i X \leq \sum_i X^* Y_i^* M^i Y_i X \\ &= X^* V^* N V X = X^* M X \leq M. \end{aligned}$$

It follows that  $Z_i Y_i X \in \mathcal{L}_M$  and  $(\mu_i X_i S, M^i) \in S_{\mathcal{F}_{T,M}}$ .

Conversely, let  $\mathcal{I}$  be the set of all  $i$  such that  $\mu_i = \text{Tr } S^* X_i^* X_i S \neq 0$  and suppose that  $(\mu_i^{-1/2} X_i S, M^i) \simeq F^i \in \mathcal{F}_{T,M}$  for all  $i \in \mathcal{I}$ . Then, for  $i \in \mathcal{I}$ ,  $F^i \simeq (\mu_{Y_i T}^{-1/2} Y_i T, M)$  for some  $Y_i \in \mathcal{L}_M$ , so that

$$S^* X_i^* M^i X_i S = s_i T^* Y_i^* M Y_i T,$$

where  $s_i = \mu_i / \mu_{Y_i}$ . Let  $M = J^* E J$  be a minimal Naimark representation of  $M$ . By Lemma 8, there are some  $C_i \in \{E\}'$ ,  $\|C_i\| \leq 1$ , such that  $C_i J = J Y_i$ ,  $i \in \mathcal{I}$ . Note that then  $J^* C_i J = J^* J Y_i = Y_i$  and  $J^* C_i^* C_i J = Y_i^* J^* J Y_i = Y_i^* Y_i$ . We then have for all  $j = 1, \dots, n$ ,

$$\begin{aligned} S^* N_j S &= \sum_{i \in \mathcal{I}} S^* X_i^* M_j^i X_i S = \sum_{i \in \mathcal{I}} s_i T^* Y_i^* M_j Y_i T = \sum_{i \in \mathcal{I}} s_i T^* Y_i^* J^* E_j J Y_i T \\ &= \sum_{i \in \mathcal{I}} s_i T^* J^* C_i^* C_i E_j J T = T^* J^* C E_j J T, \end{aligned}$$

where  $C := \sum_{i \in \mathcal{I}} s_i C_i^* C_i$ . Put  $t := \sum_i s_i$ , then  $0 \leq C \leq tI$  and  $C \in \{E\}'$ ; hence,  $D_j := t^{-1} J^* C E_j J$  satisfies  $0 \leq D_j \leq M_j$  and

$$\sum_j D_j = t^{-1} J^* C J = t^{-1} \sum_{i \in \mathcal{I}} s_i Y_i^* Y_i \in B(\mathcal{H}_0).$$

By Lemma 3, there is some  $Y \in B(\mathcal{H}_0)$  such that  $D_j = Y^* M_j Y$  and it is clear that then  $Y \in \mathcal{L}_M$ . We therefore have

$$S^* N_j S = T^* J^* C E_j J T = t T^* D_j T = t T^* Y^* M_j Y T, \quad j = 1, \dots, n,$$

so that  $(S, N) \simeq (t^{1/2} Y T, M) \in S_{\mathcal{F}_{T,M}}$ . This proves (iii).  $\square$

*Example 3.* Let  $M \in \mathcal{M}$  be a projection valued, then it is  $B(\mathcal{H}_0)$ -extremal by Corollary 1. Let  $T \in \mathcal{T}$  be surjective. It is easy to see that  $X^* M X \leq M$  if and only if  $X \in \{M\}'$ , so that the face generated by  $F$  is  $\{(\mu_X^{-1/2} X T, M), X \in B(\mathcal{H}_0) \cap \{M\}'\}$ .

We also obtain the following characterization of  $B(\mathcal{H}_0)$ -extremal POVMs.

*Corollary 2.* An element  $M \in \mathcal{M}$  is  $B(\mathcal{H}_0)$ -extremal if and only if for any surjective  $T \in \mathcal{T}$  and any convex decomposition  $F = \sum_i \lambda_i F^i$  of the corresponding process POVM  $F = T^*MT$ , we must have  $F^i \simeq (\mathcal{H}_0, S_i, M)$  for some  $S_i \in \mathcal{T}$ .

*Proof.* Assume that  $M$  is  $B(\mathcal{H}_0)$ -extremal and let  $F = \sum_i \lambda_i F^i$ . Any  $F^i$  is contained in the face of  $\mathcal{F}(\mathcal{H}, \mathcal{K}, n)$  generated by  $F$ , so that  $F^i \simeq (\mathcal{H}_0, T_i, M)$  for some  $T_i \in \mathcal{T}$ , by Proposition 2. For the converse, let  $M = \sum_i X_i^* M^i X_i$  be a proper  $B(\mathcal{H}_0)$ -convex combination and assume that  $M$  fulfills the condition. Let  $T \in \mathcal{T}$  be surjective and let  $F = T^*MT$ , then  $F = \sum_i \mu_i F^i$ , with  $F^i \simeq (\mathcal{H}_0, T_i, M^i)$  as in (9). Note that  $\mu_i > 0$  for all  $i$  since all  $X_i$  are invertible. On the other hand,  $F^i \simeq (\mathcal{H}_0, S^i, M)$  by assumption. By Lemma 6,  $M \sim_{B(\mathcal{H}_0)} M^i$  for all  $i$ . It follows that  $M$  is  $B(\mathcal{H}_0)$ -extremal.  $\square$

## V. A CHARACTERIZATION OF $\mathcal{A}$ -EXTREMAL AND $\mathcal{A}$ -PURE POVMs

In this section, we give the proofs of Lemma 2-4. We mostly follow the arguments used in the  $C^*$ -convex case. The first easy lemma and its corollary are proved similarly as, e.g., in Ref. 15.

*Lemma 11.* Let  $M \in \mathcal{M}(\mathcal{H}, n)$ ,  $M = \sum_i X_i^* M^i X_i$  be an  $\mathcal{A}$ -convex combination of  $M^1, \dots, M^m \in \mathcal{M}(\mathcal{H}, n)$ . Then, there is some  $N \in \mathcal{M}(\mathcal{H}, n)$  and  $Y_1 \in \mathcal{A}$  such that  $M = X_1^* M^1 X_1 + Y_1^* N Y_1$  is an  $\mathcal{A}$ -convex combination of  $M^1$  and  $N$ , proper if all  $X_i$  are invertible.

*Corollary 3.*  $M \in \mathcal{M}(\mathcal{H}, n)$  is  $\mathcal{A}$ -extremal if and only if whenever  $M = X M^1 X + Y M^2 Y$  for some positive invertible  $X, Y \in \mathcal{A}$ ,  $X^2 + Y^2 = I$  and  $M^1, M^2 \in \mathcal{M}(\mathcal{H}, n)$ , we must have  $M^i \sim_{\mathcal{A}} M$ .

*Proof of Lemma 2.* Here, we use similar techniques as in Ref. 7. We first prove the assertion for  $M = X_1 N^1 X_1 + X_2 N^2 X_2$ , with  $X_1, X_2 \geq 0$ . If both  $X_1$  and  $X_2$  are invertible,  $N^1, N^2 \in \mathcal{F}$  by the definition of an  $\mathcal{A}$ -face. So suppose that, say,  $X_1$  is not invertible. For any  $\lambda \in (0, 1)$ ,

$$M = X_1 N^1 X_1 + (\lambda X_2) N^2 (\lambda X_2) + (\sqrt{1 - \lambda^2} X_2) N^2 (\sqrt{1 - \lambda^2} X_2).$$

Put  $Y_\lambda = X_1^2 + (1 - \lambda^2) X_2^2 = I - \lambda^2 X_2^2$  and

$$N^\lambda := Y_\lambda^{-1/2} [X_1 N^1 X_1 + (\sqrt{1 - \lambda^2} X_2) N^2 (\sqrt{1 - \lambda^2} X_2)] Y_\lambda^{-1/2}.$$

Note that since  $X_2^2 \leq I$ ,  $Y_\lambda$  is invertible. We then have  $N^\lambda \in \mathcal{M}(\mathcal{H}, n)$  and

$$M = (\lambda X_2) N^2 (\lambda X_2) + Y_\lambda^{1/2} N^\lambda Y_\lambda^{1/2}.$$

If  $X_2$  is invertible, this is a proper  $\mathcal{A}$ -convex combination, so that  $N^2, N^\lambda \in \mathcal{F}$ . If  $X_2$  is not invertible, we repeat the same construction, with  $Y_\lambda^{1/2} N^\lambda Y_\lambda^{1/2}$  as the second element. Since  $Y_\lambda$  is invertible, we obtain  $M$  as a proper convex combination of  $N^\lambda$  and some element  $K^\lambda \in \mathcal{M}(\mathcal{H}, n)$ , so that again  $N^\lambda \in \mathcal{F}$ , and this holds for any  $\lambda \in (0, 1)$ . Since  $\mathcal{F}$  is compact, there is some sequence  $\lambda_n \rightarrow 1$ , such that  $N^{\lambda_n}$  converges to some element  $N \in \mathcal{F}$ . It follows that

$$\lim_n N^{\lambda_n} = Q_1 N^1 Q_1 + Q_1^\perp N^2 Q_1^\perp \in \mathcal{F}.$$

Let now  $A = \sum_{j=1}^m X_j^* N^j X_j$  and choose any  $j \in \{1, \dots, m\}$ . Then by Lemma 11, there is some  $K^j \in \mathcal{M}(\mathcal{H}, n)$  and  $Y_j \in \mathcal{A}$  such that  $M = X_j^* N^j X_j + Y_j^* K^j Y_j$  is an  $\mathcal{A}$ -convex combination. Let  $X_j = U_j |X_j|$ ,  $Y_j = V_j |Y_j|$  be polar decompositions, with  $U_j, V_j$  unitary elements in  $\mathcal{A}$ . Then,  $M = |X_j| M^j |X_j| + |Y_j| R^j |Y_j|$ , with  $M^j = U_j^* N^j U_j$ ,  $R^j = V_j^* K^j V_j \in \mathcal{M}(\mathcal{H}, n)$ . By the first part of the proof, for  $P_j$  the support of  $|X_j|$ ,

$$P_j M^j P_j + P_j^\perp R^j P_j^\perp = P_j U_j^* N^j U_j P_j + P_j^\perp R^j P_j^\perp \in \mathcal{F},$$

and hence, also  $Q_j N^j Q_j + Q_j^\perp L^j Q_j^\perp \in \mathcal{F}$ , where  $L^j = U_j^* R^j U_j \in \mathcal{M}(\mathcal{H}, n)$  and  $Q_j = U_j P_j U_j^*$  is the range projection of  $X_j$ .  $\square$

*Proof of Lemma 3.* Let  $M$  be  $\mathcal{A}$ -extremal and let  $0 \leq D_i \leq M_i$ ,  $\sum_i D_i =: D \in \mathcal{A}$ . Let  $Q$  be the support projection of  $D$  and let

$$N_i = D^{-1/2} D_i D^{-1/2} + \frac{1}{n} (I - Q), \quad i = 1, \dots, n.$$

Then,  $N = \{N_1, \dots, N_n\}$  is an element in  $\mathcal{M}(\mathcal{H}, n)$  and  $D_i = D^{1/2}N_iD^{1/2}$ . Similarly, let  $D'_i = M_i - D_i$ , then  $0 \leq D'_i \leq M_i$ ,  $\sum_i D'_i = I - D \in \mathcal{A}^+$  and there is some  $N' \in \mathcal{M}(\mathcal{H}, n)$  such that  $D'_i = (I - D)^{1/2}N'_i(I - D)^{1/2}$ . It follows that

$$M_i = D_i + D'_i = D^{1/2}N_iD^{1/2} + (I - D)^{1/2}N'_i(I - D)^{1/2}, \quad (12)$$

so that  $M$  is an  $\mathcal{A}$ -convex combination of  $N$  and  $N'$ . Using Lemmas 1 and 2, we obtain  $M \sim_{\mathcal{A}} QNQ + Q^\perp N'Q^\perp$ , so that there is some unitary  $U \in \mathcal{A}$  such that

$$D_i = D^{1/2}(QN_iQ + Q^\perp N'_iQ^\perp)D^{1/2} = D^{1/2}U^*M_iUD^{1/2} = X^*M_iX,$$

with  $X = UD^{1/2} \in \mathcal{A}$ .

Conversely, assume that the condition holds and let  $M = \sum_j Y_j^* M^j Y_j$  be a proper  $\mathcal{A}$ -convex combination. Then, for all  $i, j$ ,  $0 \leq Y_j^* M_i^j Y_j \leq M_i$ , hence, there is some  $X_j \in \mathcal{A}$  such that  $Y_j^* M_i^j Y_j = X_j^* M_i X_j$ . Summing over  $i$ , we obtain  $Y_j^* Y_j = X_j^* X_j$ , so that  $Y_j = U_j X_j$  for some unitary  $U_j \in \mathcal{A}$  and since  $Y_j$  is invertible, so is  $X_j$ . Hence,  $U_j^* M^j U_j = M$ , for all  $j$ , and  $M$  is  $\mathcal{A}$ -extremal.  $\square$

We now give an alternative proof of the characterization of  $C^*$ -extremal POVMs.

*Corollary 4.* Let  $M \in \mathcal{M}(\mathcal{H}, n)$ . Then,  $M$  is  $C^*$ -extremal if and only if  $M$  is projection-valued.

*Proof.* Assume that  $M$  is  $C^*$ -extremal, that is,  $\mathcal{A}$ -extremal for  $\mathcal{A} = B(\mathcal{H})$ . By Lemma 3, we obtain that whenever  $0 \leq D_i \leq M_i$ ,  $i = 1, \dots, n$ , we must have  $D_i = X^* M_i X$  for some  $X \in B(\mathcal{H})$  and summing over  $i$ , we get  $X^* X = \sum_i D_i$ . For any  $i$ , it follows by putting  $D_j = \delta_{ij} M_i$  that there is some unitary  $U_i$  such that

$$M_i^{1/2} U_i^* M_j U_i M_i^{1/2} = \delta_{ij} M_i, \quad j = 1, \dots, n.$$

Let  $Q_i = U_i \text{supp}(M_i) U_i^*$ , then for all  $j$ , we get  $Q_i M_j Q_i = \delta_{ij} Q_i$ . Hence,  $M_j \leq Q_i^\perp$  for all  $j \neq i$ , so that  $I - M_i = \sum_{j \neq i} M_j \leq Q_i^\perp$  and we must have  $M_i = Q_i$ . This proves that  $M$  is projection-valued. The converse follows by Corollary 1.  $\square$

We now turn to the characterization of  $\mathcal{A}$ -pure maps.

*Lemma 12.* Let  $\Phi : B(\mathcal{H}) \rightarrow B(\mathcal{H})$  be a unital completely positive map. Let  $\mathcal{F}_\Phi := \{X \in B(\mathcal{H}), \Phi(X) = X\}$  and let  $\mathcal{F}'_\Phi$  be the commutant of  $\mathcal{F}_\Phi$ . If  $\mathcal{F}'_\Phi = \mathbb{C}I$ , then  $\Phi = \text{id}_{\mathcal{H}}$  is the identity map on  $\mathcal{H}$ .

*Proof.* Clearly, it is enough to prove that  $\mathcal{F}_\Phi$  is a subalgebra, equivalently,  $X^* X \in \mathcal{F}_\Phi$  for any  $X \in \mathcal{F}_\Phi$ . In proving this, we follow Ref. 2, Remark 2.

Let  $\Psi$  be the pointwise limit of  $n^{-1} \sum_{k=0}^{n-1} \Phi^k$ , where  $\Phi^k = \Phi \circ \dots \circ \Phi$  is the  $k$ -fold composition. Then,  $\Psi$  is an idempotent unital completely positive map and  $\Psi \circ \Phi = \Phi \circ \Psi = \Psi$ ,  $\mathcal{F}_\Phi \subseteq \mathcal{F}_\Psi$ . Let  $Q$  be the support projection of  $\Psi$ , then by Ref. 2, Lemma 1,  $Q \in \mathcal{F}'_\Psi \subseteq \mathcal{F}'_\Phi$ , so that  $Q = I$  and  $\Psi$  is faithful. If  $X \in \mathcal{F}_\Phi$ , then by Schwarz inequality,  $X^* X = \Phi(X)^* \Phi(X) \leq \Phi(X^* X)$ . Since  $\Phi(X^* X) - X^* X \geq 0$  and  $\Psi(\Phi(X^* X) - X^* X) = \Psi(X^* X) - \Psi(X^* X) = 0$ , we have  $X^* X \in \mathcal{F}_\Phi$ .  $\square$

*Proof of Lemma 4.* Suppose  $M$  is  $\mathcal{A}$ -pure and let  $D_i \in B(P_i \mathcal{H})$  be such that  $D := \sum_i D_i \in \mathcal{A}$ . We may suppose that  $D_i$  is self-adjoint, by replacing  $D_i$  by  $\frac{1}{2}(D_i + D_i^*)$  if necessary. Moreover, there are some  $t, s \geq 0$  such that  $0 \leq tM_i + sD_i \leq M_i$  for all  $i$  and since  $\sum_i (tM_i + sD_i) = tI + sD \in \mathcal{A}$ , we may suppose  $0 \leq D_i \leq M_i$ .

By Lemma 3, there are some  $X, Y \in \mathcal{A}$  such that  $D_i = X^* M_i X$  and  $M_i - D_i = Y^* M_i Y$  for all  $i$ . Summing over  $i$ , we obtain  $X^* X + Y^* Y = I$ . Let  $\Phi(A) = X^* A X + Y^* A Y$  for  $A \in B(\mathcal{H})$ , then  $\Phi$  is a unital completely positive map and  $M_i \in \mathcal{F}_\Phi$  for all  $i$ . Clearly,  $\mathcal{A}' \subseteq \mathcal{F}_\Phi$ , so that  $\mathcal{F}'_\Phi \subseteq \mathcal{A}'' = \mathcal{A}$ . Let  $Q \in \mathcal{F}'_\Phi$  be a projection, then  $Q$  must commute with all  $M_i$ . Since  $Q \in \mathcal{A}$  and  $M$  is  $\mathcal{A}$ -pure, this implies  $Q = 0$  or  $I$ . Hence,  $\mathcal{F}'_\Phi = \mathbb{C}I$  and  $\Phi = \text{id}_{\mathcal{H}}$ , by Lemma 12. Since  $X$  and  $Y$  are Kraus operators of  $\Phi$ , we must have  $X = zI$  for some  $z \in \mathbb{C}$ ,  $|z| \leq 1$ . Thus,  $D_i = X^* M_i X = |z|^2 M_i$ ,  $i = 1, \dots, n$ .

Conversely, suppose that the condition holds, then  $M$  is  $\mathcal{A}$ -extremal by Lemma 3. If  $0 \neq P \in \mathcal{A}$  is a projection commuting with all  $M_i$ , then  $PM_i \in B(P_i \mathcal{H})$  and the condition implies that  $PM_i = \lambda M_i$  for all  $i$  and some  $\lambda \in [0, 1]$ . Hence,  $P = I$  and  $M$  is  $\mathcal{A}$ -pure.  $\square$



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