EXTREMAL COVARIANT QUANTUM OPERATIONS AND
POVM’S

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ABSTRACT. We consider the convex sets of QO’s (quantum operations) and
POVM’s (positive operator valued measures) which are covariant under a gen-
eral finite-dimensional unitary representation of a group. We derive necessary
and sufficient conditions for extremality, and give general bounds for ranks of
the extremal POVM’s and QO’s. Results are illustrated on the basis of simple
examples.

1. INTRODUCTION

The need for miniaturization and the new quantum information technology[1] has recently motivated a search for new quantum devices with maximum control at
the quantum level. Among the many problems posed by the new technology there
is the need of engineering quantum devices which perform specific measurements
or particular state transformations—the so-called quantum operations—which are optimized with respect to some given criterion. In most cases such optimal quantum measurements/operations are covariant with respect to
a group of physical transformations. For the case of a quantum measurement,
"group-covariant" means that there is an action of the group on the probability
space which maps events into events, in such a way that when the quantum system
is transformed according to a group transformation, the probability of the given
event becomes the probability of the transformed event. This situation is very
natural, and occurs in most practical applications. For example, the heterodyne
measurement[12,13] is covariant under the group of displacements of the complex
field, which means that if we displace the state of radiation by an additional complex
averaged field, then the output photo-current will be displaced by the same complex
quantity.

In quantum mechanics the probabilities for a given apparatus for all possible
states are described by positive operator valued measures (POVM)[3], and we will
say that the measurement is covariant when its POVM is covariant under a unitary
group representation[4,5]. For quantum operations (QO), on the other hand,
covariance means that the output of a group-transformed input state is simply the
transformed output state—a situation again quite common in practice. Typically
covariance means that the apparatus is required to work equally well on a full set
of states which is invariant under a group of transformations. For instance, if one
wants to engineer an eavesdropping apparatus for a BB84 cryptographic scheme
[14,15] that clones equally well all equatorial qubits, then the optimal cloning
operation must be covariant under the group $G = \mathbb{Z}_4$ of $\pi/2$ rotations of the Bloch
sphere around its polar axis, which is a subgroup of the group of all axial rotations

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Similarly, if one wants to engineer a QO which works equally well on all pure states, then the operation must be covariant under the full SU(d) group, where d is the dimension of the Hilbert space of the quantum system.

It is easy to see that all POVM’s covariant under some group representation make a convex set, which describes the complete class of possible covariant apparatuses. The same obviously holds for group-covariant QO’s. Typically in most applications the optimization resorts to minimize a concave function on the convex set of covariant machines (in quantum estimation theory actually such function is generally linear), whence the optimal machine will correspond to an extremal element of the convex set. For such purpose it is convenient to classify all extremal covariant POVM’s and QO’s, and this is precisely the subject of the present paper.

For finite dimensional Hilbert space, a characterization of all non-covariant extremal QO’s was given in Ref. [14], whereas a characterization of all extremal POVM’s can be found in Refs. [15] and [16] for discrete finite probability space. On the other hand, no classification of the extremal QO’s or POVM’s is available yet under a covariance constraint, since, as we will see, this constraint makes the classification problem much harder. Coincidentally, in many applications the optimal QO/POVM is restricted to be rank-one from the special form of the optimization function (this is the case, for example, of optimal phase estimation for pure states[2, 3, 20], or of phase covariant optimal cloning of pure states[16]), and this has lead to a widespread belief that optimality is synonym of rank-one. However, as we will see in this paper, for sufficiently large dimension the extremal QO’s/POVM’s can easily have rank larger than one: this can actually happen for optimization with mixed input states, such as in the case of optimal phase estimation with phase-coherent mixed states[21].

In this paper we provide a classification for finite dimensions of all extremal POVM’s and QO’s that are covariant under a general unitary group representation. We will generally consider continuous Lie groups, since then all results will also apply to the case of discrete groups as well, with just a little change of notation. We provide necessary and sufficient conditions for extremality, along with simple necessary conditions, which allow to "sieve" the extremal QO’s/POVM’s. From these conditions general bounds for the rank of the extremal QO’s/POVM’s easily follow as corollaries.

The paper is organized as follows. In Sect. 2 we briefly review the concept of POVM and that of covariant POVM based on the Holevo’s theorem[2]. In Section 3 we recall the necessary concepts about QO’s, including their operator form introduced in Ref. [22], which allows to easily classify the covariant QO’s as non-negative operators in the commutant of a suitable representation of the group. Section 4 is entirely devoted to some technical lemmas which will be used in the classification of both POVM’s and QO’s. Finally Sections 5 and 6 contain the classification theorem of extremal group covariant POVM’s and QO’s, respectively, with some simple explicit examples, in particular with application to phase-covariant estimation and phase-covariant optimal cloning.

2. Positive operator valued measures (POVM)

In the following we will denote by $\mathcal{B}(\mathcal{H}, \mathcal{K})$ the linear space of bounded operators from the Hilbert space $\mathcal{K}$ to the Hilbert space $\mathcal{H}$, and by $\mathcal{B}(\mathcal{H}) \equiv \mathcal{B}(\mathcal{H}, \mathcal{H})$.
the algebra of bounded operators on $\mathcal{H}$. By $\mathcal{T}_1(\mathcal{H})$ we will denote the trace-class operators on $\mathcal{H}$, and by $\mathcal{T}_1^+(\mathcal{H})$ its positive elements.

A general measurement is described by a probability space $\mathcal{X}$ equipped with a sigma-algebra structure $\sigma(\mathcal{X})$ of measurable subsets $B \in \sigma(\mathcal{X})$. The measurement returns a random outcome $x \in \mathcal{X}$. In quantum mechanics the probability that the outcome belongs to a subset $B \in \sigma(\mathcal{X})$ depends on the state $\rho \in \mathcal{T}_1^+(\mathcal{H})$ of the system in a way which is distinctive of the measuring apparatus according to the Born rule

$$p(B) = \text{Tr}[P(B)\rho],$$

where $P$ is a function on $\sigma(\mathcal{X})$ which is positive-operator valued in $\mathcal{B}(\mathcal{H})$, with the normalization condition

$$P(\mathcal{X}) = I_{\mathcal{H}}.$$

Positivity of $P$ is needed for positivity of probabilities for every state $\rho$, whereas Eq. 2 guarantees normalization of probabilities. In synthesis, $P$ is a positive operator valued measure (POVM) on the probability space $\mathcal{X}$. In a sense the POVM $P$ represents our knowledge of the measuring apparatus from which we can infer information on the state $\rho$ from probabilities. The linearity of the Born rule (1) in both arguments $\rho$ and $P$ is consistent with the intrinsically statistical nature of the measurement, in which our partial knowledge of both the system and the apparatus reflects in convex structures for both states and POVM’s. This means that not only states, but also POVM’s can be "mixed", namely there are POVM’s that give probability distributions that are equivalent to choose randomly among different apparatuses.

2.1. Group covariant POVM’s. Let’s consider now the general scenario in which a group of physical transformations $G$ can act on the probability space $\mathcal{X}$. We will write $g_{x}$ for the action of the group element $g \in G$ on the point $x \in \mathcal{X}$, and $gB$ for the action of $g$ on a whole subset $B \subseteq \mathcal{X}$. We will always consider the case in which $G$ acts transitively on $\mathcal{X}$, namely for any two points on $\mathcal{X}$ there is always a group element which connects them. A consequence of transitivity is that $\mathcal{X}$ can be always regarded as the homogeneous factor space $\mathcal{X} = G / G_x$, $G_x$ denoting the stability group of any point $x \in \mathcal{X}$.

A POVM $P$ on $\mathcal{H}$ for the probability space $\mathcal{X}$ is covariant under the unitary representation $g \rightarrow U_g$ of the group $G$ when for every set $B \in \sigma(\mathcal{X})$ one has

$$U_g^*P(B)U_g = P(g^{-1}B).$$

The following general theorem by Holevo[2] classifies all group-covariant POVM’s.

**Theorem 1** (Holevo). For square-integrable representations, a POVM $P$ on the probability space $\mathcal{X}$ is covariant with respect to the unitary representation $g \rightarrow U_g$ on $\mathcal{H}$ of the group $G$ of transformations of $\mathcal{X}$ if and only if it admits a density of the form

$$dP_z = U_{g_0}^\dagger \Xi U_{g_0} \, dx, \quad g_{x} \in G : g_{x}x_0 = x,$$

where $d\, x$ is an invariant measure on $\mathcal{X}$, with $\Xi \geq 0$ in the commutant $G'_{x_0}$ of the isotropy group $G_{x_0}$ of $x_0$, satisfying the constraint

$$\int_G d\, g U_g^\dagger \Xi U_g = I_{\mathcal{H}}.$$
with dg invariant measure on G.

In the case in which the POVM is designed to estimate the group element itself $g \in G$ corresponding to an unknown transformation $U_g$, then the stability group is the identity, whence $x = G$ and the POVM $P$ is covariant if and only if it admits a density of the form

$$d P_g = U_g^\dagger \Xi U_g d g, \quad g \in G$$

for any $\Xi \geq 0$ satisfying the constraint (5). The possible seed operators $\Xi \geq 0$ satisfying the constraint (5) form a convex set. In Section 5 we will classify all extremal elements $\Xi$ of such convex set.

3. Quantum operations

The mathematical structure that describes the most general state change in quantum mechanics—such as the evolution of an open system or the state change due to a measurement—is the quantum operation (QO) of Kraus [6, 1]. Such abstract theoretical evolution has a precise physical counterpart in its implementations as a unitary interaction between the system undergoing the QO and a part of the apparatus—the so-called ancilla—which after the interaction is read by means of a conventional quantum measurement. We can consider generally different input and output Hilbert spaces $H$ and $K$, respectively, allowing the treatment of very general quantum machines, e. g. of the kind of quantum optimal cloners [23, 22]. For example in the cloning from one to $n$ copies one has input space $H$ and output space $K = H \otimes n$, or its symmetric version $K = (H \otimes n)_{sym}$ for symmetric cloning. Within the present paper we will only consider finite dimensional Hilbert spaces. In the Heisenberg picture the QO evolves observables, and will be denoted by a map $M$ from $B(H) \rightarrow B(K)$. In the Schrödinger picture the QO evolves states, and it is given by the dual map $M^\tau : T_1(H) \rightarrow T_1(K)$, the dualism being determined by the equivalence of the two pictures in terms of the trace inner product, namely $\text{Tr}[M(X)\rho] = \text{Tr}[M^\tau(\rho)X]$ for all $\rho \in T_1(H)$ and for all $X \in B(H)$. The maps $M$ and $M^\tau$ are linear completely positive (CP), namely they preserve positivity of the input operator for any trivial extension $M \otimes I$ on a larger Hilbert space that includes any possible additional quantum system, $I$ denoting the identity map on the additional system. In the Schrödinger picture the CP property physically means that the map $M^\tau$ from $T_1(H)$ to $T_1(K)$ preserves positivity of any input state of the quantum system (with Hilbert space $H$) entangled with any possible additional quantum system. The map $M^\tau$ of a QO must also be trace-not-increasing, with the trace $\text{Tr}[M^\tau(\rho)] \leq 1$ representing the probability that the transformation occurs, and the input and output states being connected as follows

$$\rho \mapsto \rho' = \frac{M^\tau(\rho)}{\text{Tr}[M^\tau(\rho)]}.$$ 

By denoting with $I_H$ the identity operator on the Hilbert space $H$, we see that the trace-not-increasing condition along with positivity of the map are equivalent to the constraint

$$M(I_H) = K \in B(H), \quad 0 \leq K \leq I_H.$$

For finite-dimensional Hilbert spaces it is convenient to represent the maps $M$ from $B(H) \rightarrow B(H)$ as operators $R_M$ on $H \otimes H$ using the following one-to-one
correspondence
\[ R_{\mathcal{M}} = \mathcal{M}^\tau \otimes \mathcal{I}(|I\rangle \langle I|), \quad \mathcal{M}^\tau(\rho) = \text{Tr}_\mathcal{K}[ (I_\mathcal{K} \otimes \rho^\tau)R_{\mathcal{M}} ], \]
where \(|I\rangle = \sum_n |n\rangle \otimes |n\rangle\) is a fixed vector in \(\mathcal{H} \otimes \mathcal{H}\), \(\{|n\rangle \otimes |m\rangle\}\) denotes an orthonormal basis for \(\mathcal{H} \otimes \mathcal{H}\), and the transposition \(\tau\) for operators is defined with respect to the orthonormal basis \(|n\rangle\langle m|\) for \(\mathcal{B}(\mathcal{H})\) taken as real. One can easily check the correspondence \((9)\), and injectivity follows from linearity. In addition, the operator \(R_{\mathcal{M}}\) is non-negative if and only if the map \(\mathcal{M}\) is CP, and the constraint \((8)\) in terms of the operator \(K\) rewrites as follows
\[ \text{Tr}_\mathcal{H}[R_{\mathcal{M}}] = K, \quad 0 \leq K \leq I_\mathcal{K}. \]
The positive operators \(R_{\mathcal{M}}\) satisfying the constraint \((10)\) make a convex set, which is the operator counterpart of the convex set of the corresponding QO’s \(\mathcal{M}\).

3.1. Group covariant CP-maps. We call the map \(\mathcal{M}\) from \(\mathcal{B}(\mathcal{H})\) to \(\mathcal{B}(\mathcal{K})\) \(G\)-covariant, when
\[ \mathcal{M}(V_g^\dagger XV_f) = U_g^\dagger \mathcal{M}(X)U_g, \quad \forall g \in G, \]
\(\{U_g\}\) and \(\{V_g\}\) denoting unitary representations of \(G\) over the input and output spaces \(\mathcal{H}\) and \(\mathcal{K}\), respectively. The Schrödinger picture version of identity \((11)\) is
\[ \mathcal{M}^\tau(U_g \rho U_g^\dagger) = V_g \mathcal{M}^\tau(\rho) V_g^\dagger, \quad \forall g \in G, \]
where \(\mathcal{M}^\tau\) goes from \(T_1(\mathcal{H})\) to \(T_1(\mathcal{K})\).

The operator form \(R_{\mathcal{M}}\) for maps \(\mathcal{M}\) simplifies the classification of QO’s that are covariant under a group \(G\), resorting to the Wedderburn’s decomposition of the commutant of the representation. It is easy to show that the map \(\mathcal{M}\) is \(G\)-covariant (i.e. it satisfies Eq. \((11)\)) if and only if its corresponding operator \(R_{\mathcal{M}}\) is invariant under the representation \(V_g \otimes U_g^\dagger\) \([22]\). In fact, from Eq. \((9)\) using invariance of partial trace under cyclic permutation of operators acting only on the traced space one has
\[ 0 = \mathcal{M}^\tau(\rho) - V_g^\dagger \mathcal{M}^\tau(U_g \rho U_g^\dagger)V_g \]
\[ = \text{Tr}_\mathcal{H}[ (I_\mathcal{K} \otimes \rho^\tau)(R_{\mathcal{M}} - (V_g^\dagger \otimes U_g^\tau)R_{\mathcal{M}}(V_g \otimes U_g^*)] ), \]
and, since Eq. \((9)\) is a one-to-one correspondence between maps and operators, one concludes that
\[ [R_{\mathcal{M}}, V_g \otimes U_g^*] = 0, \quad \forall g \in G. \]
Therefore, the problem of classifying covariant CP-maps resorts to that of classifying positive elements of the commutant of the representation \(V_g \otimes U_g^\dagger\) on \(\mathcal{H} \otimes \mathcal{H}\). By labeling with \(k\) the generic equivalence class of the representation, with multiplicity \(m_k\), the Wedderburn’s decomposition of the representation space is written as follows \([24]\)
\[ \mathcal{H} \otimes \mathcal{H} = \bigoplus_k (\mathcal{H}_k \otimes \mathbb{C}^{m_k}). \]
Then, since \(R_{\mathcal{M}}\) must be a positive operator in the commutant of the representation it must have the general form
\[ R_{\mathcal{M}} = \oplus_k (I_\mathcal{H}_k \otimes w_k^\dagger w_k) = W^\dagger W, \quad W = \oplus_k (I_\mathcal{H}_k \otimes w_k), \]
where $w_k$ is any operator on $\mathbb{C}^{m_k}$, i.e. a $m_k \times m_k$ matrix. Therefore, the classification of covariant trace-not-increasing QO’s with $\mathcal{M}(I_X) = K \leq I_{X'}$ is equivalent to classify the operators $R_{\mathcal{M}}$ of the form (19) with the constraint
\begin{equation}
\sum_k \text{Tr}_{X'} [(I_{X_k} \otimes w_k w_k^*)] = K \leq I_{X'} .
\end{equation}

The constraint (17) is generally quite involved, due to the subspace mismatch between the tensor product $X' \otimes H$ and the Wedderburn’s decomposition: its simplification will be the main task of Section 6.

4. Technical lemmas

This section will be entirely devoted to technical lemmas, which will be used for the classification of both extremal covariant POVM’s and QO’s. The lemmas connect conditions on the vanishing of partial traces with linear spannings.

In the following we will make use of the following simple fact for any linear space $L$ and a subspace $\mathcal{I} \subseteq L$: if the only vector of $\mathcal{I}$ that is orthogonal to the whole subspace $\mathcal{I}$ is the null vector, then one has $\mathcal{I} = L$. Moreover, since orthogonality to a set $\mathcal{S}$ of vector implies orthogonality to its linear span $\text{Span}(\mathcal{S})$, then the previous assertion holds also for subsets $\mathcal{S} \subseteq L$ (not necessarily subspace), namely if the only vector orthogonal to the subset $\mathcal{S}$ is the null vector, than one has $L \equiv \text{Span}(\mathcal{S})$. From now we will also make use of the following natural notation
\begin{equation}
X(B(\mathcal{I}) \otimes I_{\mathcal{I}})Y^\dagger = \text{Span}\{X(A \otimes I_{\mathcal{I}})Y^\dagger, A \in B(\mathcal{I})\},
\end{equation}
for $X,Y$ any operators with domain $\mathcal{A} \otimes \mathcal{B}$.

**Lemma 1.** Let $B \in B(\mathcal{B}_2 \otimes \mathcal{B}_1, \mathcal{A})$, $\mathcal{A}$ and $\mathcal{B}_1, \mathcal{B}_2$ denoting arbitrary finite dimensional Hilbert spaces. Then, the injectivity of the linear CP map $\mathcal{W}(A) = \text{Tr}_{\mathcal{B}_1}[B^\dagger AB]$ on $B(\mathcal{A})$ is equivalent to the spanning condition
\begin{equation}
B(\mathcal{A}) = B(B(\mathcal{B}_2) \otimes I_{\mathcal{B}_1})B^\dagger .
\end{equation}

**Proof.** The inyectivity of the map $\mathcal{W}(A) = \text{Tr}_{\mathcal{B}_1}[B^\dagger AB]$ on $B(\mathcal{A})$ means that
\begin{equation}
\forall A \in B(\mathcal{A}) \quad \text{Tr}_{\mathcal{B}_1}[B^\dagger AB] = 0 \implies A = 0 .
\end{equation}
The condition $\text{Tr}_{\mathcal{B}_1}[B^\dagger AB] = 0$ is equivalent to $\text{Tr}[C \text{Tr}_{\mathcal{B}_1}[B^\dagger AB]] = 0 \forall C \in B(\mathcal{B}_2)$. Therefore, since one has
\begin{equation}
\text{Tr}[C \text{Tr}_{\mathcal{B}_1}[B^\dagger AB]] = \text{Tr}[C \otimes I_{\mathcal{B}_1})B^\dagger AB] = \text{Tr}[B(C \otimes I_{\mathcal{B}_1})B^\dagger A]
\end{equation}
condition (20) is then equivalent to
\begin{equation}
\forall A \in B(\mathcal{A}) \quad \text{Tr}[B(B(\mathcal{B}_2) \otimes I_{\mathcal{B}_1})B^\dagger A] = 0 \implies A = 0,
\end{equation}
where we used notation (13). Eq. (22) says that the only operator $A \in B(\mathcal{A})$ orthogonal to the operator space $B(B(\mathcal{B}_2) \otimes I_{\mathcal{B}_1})B^\dagger \subseteq B(\mathcal{A})$ is the null operator, which means that $B(B(\mathcal{B}_2) \otimes I_{\mathcal{B}_1})B^\dagger$ is actually the full linear space $B(\mathcal{A})$, namely condition (22) is equivalent to condition (19).]

The above theorem leads immediately to the following corollaries.

**Corollary 1.** A necessary condition for injectivity of the map $\mathcal{W}(A) = \text{Tr}_{\mathcal{B}_1}[B^\dagger AB]$ on $B(\mathcal{A})$ is
\begin{equation}
\dim(\mathcal{A}) \leq \min\{\dim(\mathcal{B}_2), \text{rank}(B)\}.
\end{equation}
Corollary 2. The injectivity of the map $\mathcal{W}(A) = \text{Tr}_{B_1}(B^\dagger AB)$ on $B(\mathcal{A})$ is equivalent to the existence of a linear injective map $\mathcal{V}$ from $B(\mathcal{A})$ to $B(\mathcal{B})$ such that

$$\forall A \in B(\mathcal{A}) \quad B(\mathcal{V}(A) \otimes I_{B_1})B^\dagger = A.$$  \hfill (24)

The relation between the maps $\mathcal{W}$ and $\mathcal{V}$ is given by

$$\mathcal{W}(A) = \text{Tr}_{B_1}[B^\dagger B(\mathcal{V}(A) \otimes I_{B_1})B^\dagger B].$$  \hfill (25)

Proof. The spanning condition (19)—equivalent to the injectivity of the map $\mathcal{W}(A) = \text{Tr}_{B_1}(B^\dagger AB)$ on $B(\mathcal{A})$—guarantees that for each $A \in B(\mathcal{A})$ there exists an element, say $V_A$, of $B(\mathcal{B})$ such that $B(V_A \otimes I_{B_1})B^\dagger = A$. Consider now an orthonormal basis $A_j$ for $B(\mathcal{A})$, and denote by $V_j$ any element of $B(\mathcal{B})$ such that $B(V_j \otimes I_{B_1})B^\dagger = A_j$. It is clear that the $\{V_j\}$ can be chosen as linearly independent. Now, for every element $A \in B(\mathcal{A})$ define $\mathcal{V}(A) = \sum_j \text{Tr}[A^\dagger_j A]V_j$. This map is clearly linear and injective. The map $\mathcal{V}(A)$ corresponds to a nonorthogonal change of basis (from $\{A_j\}$ to $\{V_j\}$) which compensates the nonorthogonal change of basis $B(V_j \otimes I_{B_1})B^\dagger = A_j$. Eq. (25) follows by substituting Eq. (24) into the map $\mathcal{W}$. \hfill \qed

We have also the additional lemma.

Lemma 2. As in Lemma 1, the injectivity of the map $\mathcal{W}(A) = \text{Tr}_{B_1}(B^\dagger AB)$ on $B(\mathcal{A})$ is equivalent to the linear independence of the set of operators $\{W_i^\dagger W_j\}$, where $W_i \in B(\mathcal{B}_1, \mathcal{B}_2)$ are defined from the singular value decomposition $B = \sum_i |V_i\rangle \langle W_i|$ through the identity $|W_i\rangle = (W_i \otimes I_{\mathcal{B}_1})|I\rangle$, $|I\rangle \in \mathcal{B}_1^{\otimes 2}$ denoting the fixed vector $|I\rangle = \sum_i |i\rangle \otimes |i\rangle$, for $\{|i\rangle \otimes |m\rangle\}$ arbitrary orthonormal basis of $\mathcal{B}_1^{\otimes 2}$.

Proof. First, notice that the identity $|X\rangle = (X \otimes I_{\mathcal{B}_1})|I\rangle$ sets a bijection between vectors $|X\rangle \in \mathcal{B}_2 \otimes \mathcal{B}_1$ and operators $X \in B(\mathcal{B}_1, \mathcal{B}_2)$. Then, using the singular value decomposition $B = \sum_i |V_i\rangle \langle W_i|$, with $|V_i\rangle \in \mathcal{A}$ and $|W_i\rangle \in \mathcal{B}_2 \otimes \mathcal{B}_1$, the partial trace in Eq. (20) becomes

$$\text{Tr}_{\mathcal{B}_1}[B^\dagger AB] = \sum_{ij} \langle W_j|\langle V_i|A|V_j\rangle \text{Tr}_{\mathcal{B}_1}[\tau(W_i)]W_j^\dagger W_j^*,$$  \hfill (26)

where $\tau$ denotes the transposition for which $(X \otimes I_{\mathcal{B}_1})|I\rangle = (I_{\mathcal{B}_1} \otimes X^\tau)|I\rangle$, and $^*$ denotes complex conjugation, i. e. $X^\dagger = (X^\tau)^*$. By taking the complex conjugate of the last equation and introducing the matrix $A_{ij} = \langle V_i|A|V_j\rangle^* \in \mathcal{M}_N(\mathbb{C})$ where $N = \text{rank}(B)$ ($N^2$ is the cardinality of the set $\{W_i^\dagger W_j\}$), the statement (26) is equivalent to

$$\{A_{ij}\} \in \mathcal{M}_N(\mathbb{C}), \quad \sum_{ij} A_{ij}W_i^\dagger W_j = 0 \implies A_{ij} = 0, \quad \forall i,j,$$  \hfill (27)

namely the operators $\{W_i^\dagger W_j\}$ are linearly independent. \hfill \qed

In the following we will need the following generalization of Lemma 1.

Lemma 3. Let $B \in B(\oplus_k (\mathcal{B}_2^{(k)} \otimes \mathcal{B}_1^{(k)}), \mathcal{A})$, and denote by $P_k$ the orthogonal projector over $\mathcal{B}_2^{(k)} \otimes \mathcal{B}_1^{(k)}$, $\mathcal{A}$ and $\mathcal{B}_1^{(k), k}$ being arbitrary finite-dimensional Hilbert spaces.
The following implication
\begin{equation}
A \in \mathcal{B}(\mathcal{A}), \quad \text{Tr}_{\mathcal{A}_2^k}[P_kB^\dagger ABP_k] = 0 \quad \forall k \implies A = 0.
\end{equation}
is equivalent to
\begin{equation}
\mathcal{B}(\mathcal{A}) = \text{Span}\{B[\oplus_k (\mathcal{B}_2^k) \otimes I_{\mathcal{A}_1^k})]B^\dagger\},
\end{equation}
and necessary conditions are
\begin{align}
\dim(\mathcal{A})^2 & \leq \sum_k \dim(\mathcal{B}_2^k)^2, \\
\dim(\mathcal{A}) & \leq \text{rank}(B).
\end{align}

**Proof.** The condition \( \text{Tr}_{\mathcal{A}_2^k}[P_kB^\dagger ABP_k] = 0 \quad \forall k \) is equivalent to say that for any \( C_k \in \mathcal{B}(\mathcal{A}_2^k) \) one has \( \text{Tr}[P_kC_k \text{Tr}_{\mathcal{A}_1^k}[P_kB^\dagger ABP_k]] = 0 \quad \forall k \). Since one has
\begin{align}
\text{Tr}[C_k \text{Tr}_{\mathcal{A}_1^k}[P_kB^\dagger ABP_k]] &= \text{Tr}[(C_k \otimes I_{\mathcal{A}_1^k})P_kB^\dagger ABP_k] \\
&= \text{Tr}[BP_k(C_k \otimes I_{\mathcal{A}_1^k})P_kB^\dagger A],
\end{align}
and, therefore, condition (28) is equivalent to
\begin{equation}
A \in \mathcal{B}(\mathcal{A}), \quad \text{Tr}[BP_k(\mathcal{B}(\mathcal{A}_2^k) \otimes I_{\mathcal{A}_1^k})P_kB^\dagger A] = 0 \quad \forall k \implies A = 0.
\end{equation}
The last condition says that the only operator in \( \mathcal{B}(\mathcal{A}) \) which is orthogonal to the set \( BP_k(\mathcal{B}(\mathcal{A}_2^k) \otimes I_{\mathcal{A}_1^k})P_kB^\dagger \quad \forall k \) is the null operator, or, in other words that the set spans the full operator space \( \mathcal{B}(\mathcal{A}) \), namely Eq. (29). The necessary conditions then follow trivially. ■

We are now ready to classify the extremal group covariant POVM’s and QO’s in the following sections. In order to classify extremal elements of convex sets, we will use the method of perturbations. We will call a non null operator \( B \) a perturbation for an operator \( A \) in a convex set if both \( A \pm tB \) are still in the convex set for some (sufficiently small) \( t > 0 \). Then, clearly \( A \) is not extremal in the convex set if and only if it has a perturbation.

### 5. Extremal covariant POVM’s

We have seen that the covariant POVM for the estimation of a group element \( g \) of an unknown unitary transformation \( U_g \) is of the general form
\begin{equation}
dP_g = d g U_g^\dagger \Xi U_g^\dagger,
\end{equation}
with probability space \( \mathcal{X} = \mathbf{G} \), and with
\begin{equation}
\int_{\mathbf{G}} d g U_g^\dagger \Xi U_g = I_\mathcal{H}.
\end{equation}
The Wedderburn’s decomposition (13) of the representation space here rewrites as follows
\begin{equation}
\mathcal{H} = \bigoplus_k (\mathcal{H}_k \otimes \mathbb{C}^{m_k}),
\end{equation}
where we remind that \( k \) labels the equivalence class of irreducible components, and \( m_k \) denotes its multiplicity. The integral in the normalization condition (35)
belongs to the commutant of the representation, whence it can be rewritten as follows

\[ \int g U_g^\dagger U_g = \bigoplus_k d_{\mathcal{H}_k}^{-1} \left[ I_{\mathcal{H}_k} \otimes \text{Tr}_{\mathcal{H}_k}(P_k \Xi P_k) \right] = I_{\mathcal{H}}, \]

where \( P_k \) denotes the orthogonal projector on the subspace \( \mathcal{H}_k \otimes \mathbb{C}^{m_k} \). Eq. \((37)\) follows from the simple fact that for an irreducible representation on the space say \( \mathcal{L} \), one has \( \int g d U_g^\dagger Z U_g = d_Z^{-1} \text{Tr}[Z] I_{\mathcal{L}} \) for measure \( d g \) normalized to unit on \( \mathcal{G} \). Eq. \((37)\) allows to split the constraint \((35)\) into the following set of constraints

\[ \text{Tr}_{\mathcal{H}_k}(P_k \Xi P_k) = d_{\mathcal{H}_k} I_{m_k}, \quad \forall k, \]

where \( I_{m_k} \) we denote the identity matrix over \( \mathbb{C}^{m_k} \). We then conclude that the classification of extremal \( \mathcal{G} \)-covariant POVM’s is equivalent to find the extremal \( \Xi \) within the convex set of operators \( \Xi \geq 0 \) satisfying the constraints \((38)\). For such purpose we have the following theorem.

**Theorem 2.** Let \( \Xi \) be an element of the convex set of positive operators on \( \mathcal{H} \) satisfying the constraints

\[ \text{Tr}_{\mathcal{H}_k}(P_k \Xi P_k) = d_{\mathcal{H}_k} I_{m_k}, \quad \forall k \in S, \]

where \( S \) denotes the set of equivalence classes of irreducible components in the representation. Write \( \Xi \) in the form \( \Xi = X^\dagger AX \) with \( A \geq 0 \), choosing \( \text{Rng}(X) = \text{Supp}(A) \cap \text{Ker}(A)^\perp \). Then

1. \( \Theta \) is a perturbation of \( \Xi \) if and only if \( \Theta \) is Hermitian, with \( \text{Tr}_{\mathcal{H}_k}(P_k \Theta P_k) = 0 \) \( \forall k \in S \), and \( \Theta = X^\dagger BX \) for some nonzero Hermitian \( B \) with \( \text{Supp}(B) \subseteq \text{Supp}(A) \).

2. For the specific choice of the form of \( A = \oplus_k A_k \), with \( A_k \in \mathcal{B}(\mathcal{H}_k \otimes \mathbb{C}^{m_k}) \), one has \( B = \oplus_k B_k \), \( B_k \in \mathcal{B}(\mathcal{H}_k \otimes \mathbb{C}^{m_k}) \) and \( \text{Supp}(B_k) \subseteq \text{Supp}(A_k) \), \( \forall k \in S \).

3. \( \Xi = X^\dagger X \) is extremal if and only if

\[ B(\text{Rng}(X)) = \text{Span}\{X \oplus_k (I_{\mathcal{H}_k} \otimes \mathbb{C}^{m_k})]\} X^\dagger \} \}

**Proof.**

1. Let \( \Theta \) Hermitian, with \( \text{Tr}_{\mathcal{H}_k}(P_k \Theta P_k) = 0 \), and \( \Theta = X^\dagger BX \) for some nonzero Hermitian \( B \in \mathcal{B}(\mathcal{H}) \) and with \( \text{Supp}(B) \subseteq \text{Supp}(A) \). Then for \( \text{rank}(B) > 0 \) \( \Theta \) is necessarily nonzero, and since \( A \geq 0 \), both constraints \( A \pm tB \geq 0 \) and \( \text{Tr}_{\mathcal{H}_k}(P_k(\Xi \pm t\Theta)P_k) = d_{\mathcal{H}_k} I_{m_k} \) \( \forall k \) are satisfied for some \( t > 0 \), whence \( \Theta \) is a perturbation for \( \Xi \). Conversely, suppose \( \Theta \in \mathcal{B}(\mathcal{H}) \) is a perturbation for \( \Xi \). Since we must have \( \Xi \pm t\Theta \geq 0 \) and \( \text{Tr}_{\mathcal{H}_k}(P_k(\Xi \pm t\Theta)P_k) = d_{\mathcal{H}_k} I_{m_k} \) for some \( t > 0 \), then \( \Theta \) is Hermitian with \( \text{Tr}_{\mathcal{H}_k}(P_k(\Theta P_k)) = 0 \) \( \forall k \in S \). Moreover, if we write \( \Xi \) in the form \( \Xi = X^\dagger AX \) with nonnegative \( A \in \mathcal{B}(\mathcal{H}) \), and \( \text{Rng}(X) = \text{Supp}(A) \), then also \( \Theta \) can be written in the same form \( \Theta = X^\dagger BX \) for some nonzero Hermitian \( B \in \mathcal{B}(\mathcal{H}) \) and \( \text{Tr}_{\mathcal{H}_k}[P_k(\Xi \pm t\Theta)P_k] = d_{\mathcal{H}_k} I_{m_k} \). In fact, if \( X \) is not invertible, it can be always completed to an invertible operator \( Z = X + Y \) by adding an operator \( Y \) with \( \text{Rng}(Y) = \text{Ker}(A) \), and one can equivalently write \( \Xi = Z^\dagger AZ \). Now we can write also the perturbation operator in the form \( \Theta = Z^\dagger BZ \). However, since \( A \pm tB \geq 0 \) for some \( t \), then necessarily \( B \) must have \( \text{Supp}(B) \subseteq \text{Supp}(A) = \text{Rng}(X) \), whence \( Z^\dagger BZ = X^\dagger BX \).

2. First it is obvious that a choice of the form \( A = \oplus_k A_k \), with \( A_k \in \mathcal{B}(\mathcal{H}_k \otimes \mathbb{C}^{m_k}) \) is always possible. Then, in order to have \( A \pm tB \geq 0 \) for some \( t > 0 \), one must have \( B = \oplus_k B_k \), each \( B_k \) Hermitian, with \( \text{Supp}(B_k) \subseteq \text{Supp}(A_k) \), \( \forall k \in S \).
3. Since \( \text{Supp}(A) \subseteq \text{Rng}(X) \) and \( A \geq 0 \), we can always merge \( \sqrt{A} \) into \( X \) by substituting \( X \rightarrow \sqrt{A}X \). Then, since \( \Xi \) is not extremal if it has a perturbation, by part 1 one sees that \( \Xi \) is extremal if for Hermitian \( B \in \mathcal{B}(\mathcal{H}) \) with \( \text{Supp}(B) \subseteq \text{Rng}(X) \), one has

\[
(41) \quad \text{Tr}_{\mathcal{H}_k}(P_kX^\dagger BX^\dagger P_k) = 0 \quad \forall k \in S \quad \implies \quad B = 0,
\]

whence via Cartesian decomposition of \( B \) we have the equivalent statement

\[
(42) \quad B \in \mathcal{B}(\text{Rng}(X)), \quad \text{Tr}_{\mathcal{H}_k}(P_kX^\dagger BX^\dagger P_k) = 0 \quad \forall k \in S \quad \implies \quad B = 0.
\]

Then, by Lemma 2 this is equivalent to condition (10). 

**Corollary 3.** A necessary condition for extremality of the seed \( \Xi \) of a group covariant representation as in Theorem 2 is

\[
(43) \quad \text{rank}(\Xi)^2 \leq \sum_k m_k^2.
\]

**Proof.** Eq. (43) is a trivial consequence of the necessary condition (10).

**Corollary 4.** Every rank-one POVM is extremal.

**Proof.** For \( \text{rank}(X) = 1 \) the iff condition (10) is trivially satisfied.

**Theorem 3.** For \( S \) containing only a single equivalence class, say \( h \), with multiplicity \( m_h \geq 1 \), the extremality of a covariant POVM on the Hilbert space \( \mathcal{H} = \mathcal{H}_h \otimes \mathbb{C}^{m_h} \) is equivalent to the linear independence of the set of operators \( \{W_i \}_{i \in S} \), where \( W_i \in \mathcal{B}((\mathbb{C}^{m_h}), \mathcal{H}_h) \) are defined from the spectral decomposition \( \Xi = \sum_i |W_i\rangle\langle W_i| \) of the seed \( \Xi \) of the POVM through the identity \( |W_i\rangle = (W_i \otimes I_{m_h})|I\rangle \), \( |I\rangle \in (\mathbb{C}^{m_h})^\otimes 2 \) denoting the fixed vector \( |I\rangle = \sum_i |l\rangle \otimes |l_i\rangle \), for \( \{ |l\rangle \otimes |m_i\rangle \} \) arbitrary orthonormal basis of \( (\mathbb{C}^{m_h})^\otimes 2 \). Extremal POVM’s with any rank \( \text{rank}(\Xi) \leq m_h \) are admissible.

**Proof.** For \( S \) containing a single equivalence class \( h \) with multiplicity \( m_h \geq 1 \) the seed \( \Xi \) of the POVM must satisfy the single constraint

\[
(44) \quad \text{Tr}_{\mathcal{H}_h}(\Xi) = d_{\mathcal{H}_h} I_{m_h}. \]

Now, write \( \Xi \) in the form \( \Xi = X^\dagger AX \) with \( X \in \mathcal{B}(\mathcal{H}_h \otimes \mathbb{C}^{m_h}, \mathfrak{A}) \), and \( \text{Rng}(X) = \text{Supp}(A) \), \( \mathfrak{A} \) being a Hilbert space such that \( \text{Supp}(A) \subseteq \mathfrak{A} \subseteq \mathcal{H}_h \otimes \mathbb{C}^{m_h} \), and which can be chosen as \( \mathfrak{A} \cong \text{Rng}(X) \). Then, according to Theorem 2 \( \Theta \) is a perturbation for \( \Xi \) if and only if it is of the form \( \Theta = X^\dagger BX \), with \( B \) Hermitian, \( \text{Supp}(B) \subseteq \text{Supp}(A) \), and \( \text{Tr}_{\mathcal{H}_h}(X^\dagger BX) = 0 \). This means that the extremality of \( \Xi \) is equivalent to the injectivity of the map \( \mathcal{W}(B) = \text{Tr}_{\mathcal{H}_h}(X^\dagger BX) \) over the set of Hermitian operators \( B \) with \( \text{Supp}(B) \subseteq \text{Supp}(A) \), which is equivalent to injectivity of the same map on \( \mathcal{B}((\text{Rng}(X))) \). We are thus in the situation of Lemma 2 with \( \mathfrak{A} = \text{Rng}(X) \), \( \mathcal{B}_1 = \mathbb{C}^{m_h} \) and \( \mathcal{B}_2 = \mathcal{H}_h \). Therefore, by writing the singular value decomposition of \( X = \sum_i |V_i\rangle\langle W_i| \), with \( \text{Span}(|V_i\rangle) = \text{Rng}(X) = \text{Supp}(A) \) the injectivity of the map \( \mathcal{W}(B) = \text{Tr}_{\mathcal{H}_h}(X^\dagger BX) \) on \( B(\text{Rng}(\mathfrak{A})) \) is equivalent to the linear independence of the set of operators \( \{W_i \}_{i \in S} \), where \( W_i \in \mathcal{B}(\mathbb{C}^{m_h}, \mathcal{H}_h) \) are defined through the identity \( |W_i\rangle = (W_i \otimes I_{m_h})|I\rangle \), \( |I\rangle \in (\mathbb{C}^{m_h})^\otimes 2 \) denoting the fixed vector \( |I\rangle = \sum_i |l\rangle \otimes |l_i\rangle \), with \( \{ |l\rangle \otimes |m_i\rangle \} \) arbitrary orthonormal basis of \( (\mathbb{C}^{m_h})^\otimes 2 \). Now, the maximum rank of the POVM is given by the maximum number of operators \( W_i \) such that the set of operators \( \{W_i \}_{i \in S} \) in \( \mathcal{B}(\mathbb{C}^{m_h}) \) is linearly independent. Since we can have at most \( m_h^2 \) linearly independent operators in \( \mathcal{B}(\mathbb{C}^{m_h}) \), the maximum cardinality of the set \( \{W_i \} \) is \( m_h \).
Corollary 5. A POVM which is covariant under an irreducible representation is extremal iff it is rank one.

Proof. For \( S \) containing a single equivalence class \( h \) with multiplicity \( m_h = 1 \) the iff condition (40) rewrites

\[
\mathcal{B}(\text{Rng}(X)) = \text{Span}\{X(I_{\mathcal{H}(h)} \otimes \mathbb{C}^1)X^\dagger\} = \text{Span}\{XX^\dagger\},
\]

which is satisfied iff \( \text{rank}(X) = 1 \). As an alternative proof, the present corollary corresponds to the situation of Theorem 3 for multiplicity \( m_h = 1 \).

5.1. Example. Consider a POVM on \( \mathcal{H} \) with \( \text{dim}(\mathcal{H}) = d \) covariant under \( G = U(1) \), with

\[
U_\phi = \exp(i\phi N), \quad N = \sum_{n=0}^{d-1} n|n\rangle\langle n|.
\]

Here we have \( d \) one-dimensional irreducible representations with characters \( \chi_k(\phi) = \exp(ik\phi) \), \( k = 0, \ldots, d-1 \), namely they are all inequivalent, whence with unit multiplicity. Therefore, the necessary condition (43) bounds the rank of the POVM as follows

\[
\text{rank}(\Xi)^2 \leq \text{dim}(\mathcal{H}),
\]

and in order to have \( \text{rank}(\Xi) = 2 \) one must have \( \text{dim}(\mathcal{H}) \geq 4 \). According to Theorem 2 the extremal POVM’s have seed of the form \( \Xi = X^\dagger X \) satisfying the identity

\[
\mathcal{B}(\text{Rng}(X)) = \text{Span}\{|X_k\rangle\langle X_k| : 0 \leq k \leq \text{dim}(\mathcal{H})\},
\]

where \( |X_k\rangle = X|k\rangle \), \( \{ |k\rangle \} \) denoting any orthonormal basis for \( \mathcal{H} \). Notice that in the present example the operator \( \Xi \) corresponds to a so-called correlation matrix, namely a positive matrix with all ones on the diagonal. This follows from the constraint (38), which in our case is simply \( \langle k|\Xi|k\rangle = 1, \forall k \). Therefore, the present classification of extremal POVM’s coincides with the classification of extremal correlation matrices given in Ref. [25].

5.2. Example. Consider a POVM for \( n \) qubits on the Hilbert space \( \mathcal{H} = (\mathbb{C}^2)^{\otimes n} \) covariant under the tensor representation \( U_\phi \otimes \mathbb{I} \) of \( G = U(1) \), with

\[
U_\phi = \exp(i\phi 1|1\rangle\langle 1|),
\]

where \( \{ |0\rangle, |1\rangle \} \) is an orthonormal basis for \( \mathbb{C}^2 \). Here we have \( n + 1 \) one-dimensional irreducible representations with characters \( \chi_k(\phi) = \exp(ik\phi) \), \( k = 0, \ldots, n \), and with multiplicity \( m_k = \binom{n}{k} \). An orthonormal basis of each subspace \( \mathbb{C}^{m_k} \) of \( \mathcal{H} = \bigoplus_k \mathbb{C}^{m_k} \) is given by

\[
\{ |j\rangle_k \} = \{ P_j^{(n,k)}|00\ldots011\ldots1\rangle_{n-k}^k \},
\]

where \( P_j^{(n,k)} \) denotes the \( j \)th permutation of \( k \) qubits in the state \( |1\rangle \) in the tensor product of \( n \) qubits in total, with all other qubits in the state \( |0\rangle \). In the present example, the iff condition for extremality (40) requires that \( \Xi = X^\dagger X \) satisfies the identity

\[
\mathcal{B}(\text{Rng}(X)) = \text{Span}\{X^\dagger X|k\rangle\langle k|X, k \in S, i, j = 1, \ldots m_k\},
\]
where now \( \{|i\rangle_k\} \) denotes any orthonormal basis for \( \mathbb{C}^{m_k} \). The necessary condition bounds the rank of the POVM as follows
\[
\text{rank}(\Xi)^2 \leq \sum_{k=0}^{n} \binom{n}{k}^2 = \left(\frac{2n}{n}\right).
\]
Here, in order to have \( \text{rank}(\Xi) \geq 2 \) one needs \( n \geq 2 \) qubits. For \( n = 2 \) according to the previous example, one necessarily must have at least two inequivalent classes, since each of the irreducible components has less than four dimensions (the same is true also for \( n = 3 \)). The previous example is also recovered by considering the special case in which \( \text{Rng}(X) \subseteq \left(\mathbb{C}^2\right)^n_+ \) i. e. containing only the sub-representation of \( U_\phi \otimes^{n} \) on the symmetric subspace \( \left(\mathbb{C}^2\right)^n_+ \), with multiplicity 1.

5.3. Example. Consider a POVM on \( \mathcal{H} \otimes \mathbb{C}^2 \) which is covariant under the group representation \( U_g \otimes I_{\mathcal{H}} \), where \( U_g \) is an irreducible representation of \( G \) on \( \mathcal{H} \). Here, we trivially have a single equivalence class, say \( h \), (corresponding to the irreducible representation \( U_g \)) with multiplicity \( m_h = \text{dim}(\mathcal{H}) \), i. e. the Hilbert space \( \mathcal{H} \) coincides with the multiplicity space \( \mathcal{H} \simeq \mathbb{C}^{m_h} \). This is exactly the case considered in Theorem 3. Therefore, the extremality of the POVM is equivalent to the linear independence of the set of operators \( \{W_i^\dagger W_j\} \), where \( W_i \in B(\mathcal{H}) \) are defined from the spectral decomposition \( \Xi = \sum_i |W_i\rangle\langle W_i| \) of the seed \( \Xi \) of the POVM through the identity \( |W_i\rangle = (W_i \otimes I_{\mathcal{H}})|I\rangle \), as in Theorem 3. Therefore, we can have extremal POVM’s with any \( \text{rank}(\Xi) \leq \text{dim}(\mathcal{H}) \). Notice that there cannot be more than a single maximally entangled vector \( |W_i\rangle \) in the decomposition of \( \Xi \), since, otherwise, at least two operators \( W_i \) would be proportional to unitary operators, and then the set \( \{W_i^\dagger W_j\} \) would be necessarily linearly dependent (two products would be both proportional to the identity). The rank-one case with a single maximally entangled projector corresponds to a so-called Bell POVM.

6. Extremal covariant quantum operations

In the following we will denote shortly by \( \mathcal{A}_G \) the operator algebra generated by the group representation \( V_g \otimes U^*_g \), by \( \mathcal{A}_G^\prime \) its commutant, and finally by \( \mathcal{H}_G \) the Hermitian operators in the commutant. The following theorem classifies all extremal \( G \)-covariant maps \( \mathcal{M} \) in the convex set given by Eq. (17).

**Theorem 4.** Let \( R \) be an element of the convex set of positive operators in the commutant \( \mathcal{A}_G^\prime \) of the operator algebra \( \mathcal{A}_G \) generated by the group representation \( V_g \otimes U^*_g \) on \( \mathcal{H} \otimes \mathcal{H} \), i. e. of the form
\[
R = \oplus_k (I_{\mathcal{H}_k} \otimes w_k^\dagger w_k) = W^\dagger W, \quad W = \oplus_k (I_{\mathcal{H}_k} \otimes w_k),
\]
satisfying the constraint
\[
\sum_k \text{Tr}_{\mathcal{H}} [(I_{\mathcal{H}_k} \otimes w_k^\dagger w_k)] = K \leq I_{\mathcal{H}},
\]
where
\[
\mathcal{H} \otimes \mathcal{H} = \bigoplus_k (\mathcal{H}_k \otimes \mathbb{C}^{m_k})
\]
is the Wedderburn’s decomposition of the representation space, \( k \) labeling the equivalence class of representations, with multiplicity \( m_k \). Denote by \( P_k \) the orthogonal...
projector over the space $\mathcal{H}_k \otimes \mathbb{C}^{m_k}$ of the equivalence class. Write $R$ in the form $R = X^\dagger QX$ with $Q, X \in \mathcal{A}_G'$ and $\text{Rng}(X) = \text{Supp}(Q)$. Then:

1. $S$ is a perturbation of $R$ if and only if $S \in \mathcal{H}_G$, with $\text{Tr}_{\mathcal{X}}[S] = 0$, and $S = X^\dagger OX$ for some nonzero $O \in \mathcal{H}_G$ with $\text{Supp}(O) \subseteq \text{Rng}(X)$. Specifically, writing $Q = \oplus_k (I_{\mathcal{H}_k} \otimes Q_k)$ and $X = \oplus_k (I_{\mathcal{H}_k} \otimes X_k)$, one has $O = \oplus_k (I_{\mathcal{H}_k} \otimes O_k)$ with $\text{Supp}(O_k) \subseteq \text{Rng}(X_k) \quad \forall k$.

2. One can always write $R$ in the form $R = X^\dagger X$, with $X \in \mathcal{A}_G'$ of the form $X = \oplus_k (I_{\mathcal{H}_k} \otimes X_k)$. Denote by $S$ the set of equivalence classes $k$ for which $X_k \neq 0$. Then, a necessary and sufficient condition for extremality of $R = X^\dagger X$ with $\text{Tr}_{\mathcal{X}}[R] = K$ is the injectivity of the map $\mathcal{F}(O) = \text{Tr}_{\mathcal{X}}[X^\dagger OX]$ on $\mathcal{A}_G' \cap \mathcal{B}(\text{Rng}(X))$, namely

$$O \in \mathcal{A}_G' \cap \mathcal{B}(\text{Rng}(X)), \quad \text{Tr}_{\mathcal{X}}[X^\dagger OX] = 0 \implies O = 0,$$

which is equivalent to

$$\bigoplus_{k \in S} \mathcal{B}(\text{Rng}(X_k)) = \bigoplus_{k \in S} X_k \text{Tr}_{\mathcal{H}_k} [P_k (I_{\mathcal{H}_k} \otimes \mathcal{B}(\mathcal{H})) P_k] X_k^\dagger. \quad (57)$$

Proof.

1. Let $S \in \mathcal{H}_G$, with $\text{Tr}_{\mathcal{X}}[S] = 0$, and $S = X^\dagger OX$ for some nonzero Hermitian $O$ with $\text{Supp}(O) \subseteq \text{Supp}(Q)$. Then for $\text{rank}(O) > 0$ $S \in \mathcal{H}_G'$ is necessarily nonzero, and since $\mathcal{H}_G' \ni Q \geq 0$, all constraints: $Q \pm tO \in \mathcal{H}_G'$, $Q \pm tO \geq 0$, and $\text{Tr}_{\mathcal{X}}[R \pm tS] = K$ are satisfied for some $t > 0$, whence $S$ is a perturbation for $R$. Conversely, suppose that $S \in \mathcal{H} \otimes \mathcal{H}$ is a perturbation for $R$. Since we must have $\mathcal{H}_G' \ni R \pm tS \geq 0$ and $\text{Tr}_{\mathcal{X}}[R \pm tS] = K$ for some $t > 0$, then $S \in \mathcal{H}_G'$ with $\text{Tr}_{\mathcal{X}}[S] = 0$. Moreover, if we write $R$ in the form $R = X^\dagger QX$ with $\text{Rng}(X) = \text{Supp}(Q)$, then also $S$ can be written in the form $S = X^\dagger OX$ for some nonzero Hermitian $O \in \mathcal{H}_G'$.

In fact, if $X$ is not invertible, it can be always completed to an invertible operator $Z = X + Y$ by adding an operator $Y \in \mathcal{A}_G'$ of the form $Y = \oplus_k (I_{\mathcal{H}_k} \otimes Y_k)$ with $\text{Rng}(Y_k) = \text{Ker}(Q_k)$ (where $Q = \oplus_k (I_{\mathcal{H}_k} \otimes Q_k)$), and one can equivalently write $R = Z^\dagger QZ$ with $Q \in \mathcal{H}_G'$ and $Z \in \mathcal{A}_G'$. Now we can write also the perturbation operator in the form $S = Z^\dagger OZ$. However, since for some $t$ the operator $Q \pm tO \geq 0$ must belong to the commutant $\mathcal{A}_G'$, then necessarily $O \in \mathcal{H}_G'$ and $\text{Supp}(O) \subseteq \text{Supp}(Q) = \text{Rng}(X)$, with $Z^\dagger OZ = X^\dagger OX$. Specifically, writing $Q = \oplus_k (I_{\mathcal{H}_k} \otimes Q_k)$, one has $O = \oplus_k (I_{\mathcal{H}_k} \otimes O_k)$ with $\text{Supp}(O_k) \subseteq \text{Supp}(Q_k) = \text{Rng}(X_k) \quad \forall k$.

2. As in part 1 we can always take $Q$ as the identity, and redefine $X = \sqrt{Q}X$, since $Q \geq 0$, keeping $X$ of the form $X = \oplus_k (I_{\mathcal{H}_k} \otimes X_k)$, since both operators in the product $\sqrt{Q}X$ belong to the algebra $\mathcal{A}_G'$. From part 1 we then see that $R = X^\dagger X$ with $X \in \mathcal{A}_G'$ is extremal if and only if

$$O \in \mathcal{H}_G' \cap \mathcal{B}(\text{Rng}(X)), \quad \text{Tr}_{\mathcal{X}}[X^\dagger OX] = 0 \implies O = 0,$$

and via Cartesian decomposition this is equivalent to

$$O \in \mathcal{A}_G' \cap \mathcal{B}(\text{Rng}(X)), \quad \text{Tr}_{\mathcal{X}}[X^\dagger OX] = 0 \implies O = 0. \quad (59)$$

Since $O \in \mathcal{A}_G' \cap \mathcal{B}(\text{Rng}(X))$ can be decomposed as $O = \oplus_k (I_{\mathcal{H}_k} \otimes O_k)$ with $O_k \in \mathcal{B}(\text{Rng}(X_k)) \quad \forall k \in S$, then the statement (59) is equivalent to

$$\forall k \in S \quad O_k \in \mathcal{B}(\text{Rng}(X_k)), \quad \sum_{k \in S} \text{Tr}_{\mathcal{X}}[(I_{\mathcal{H}_k} \otimes X_k)^\dagger (I_{\mathcal{H}_k} \otimes O_k)(I_{\mathcal{H}_k} \otimes X_k)] = 0 \implies O_k = 0 \forall k \in S, \quad (60)$$
or else

(61) \[ \forall k \in S \quad O_k \in B(\text{Rng}(X_k)), \]

\[ \text{Tr}_{\mathcal{X}}[\oplus_{k \in S}(I_{\mathcal{X}} \otimes X_k)(I_{\mathcal{X}} \otimes O_k)(I_{\mathcal{X}} \otimes X_k)] = 0 \implies O_k = 0 \forall k \in S, \]

The vanishing of the partial trace can be written as the vanishing of the trace

(62) \[ \text{Tr}\{\oplus_{k \in S}X_k \text{Tr}_{\mathcal{X}}[P_k(I_{\mathcal{X}} \otimes B(\mathcal{H}))P_k]X_k^\dagger\} = 0 \implies S = 0, \]

namely, since the only operator in the linear space \( \oplus_{k \in S}B(\text{Rng}(X_k)) \) orthogonal to the subspace \( \oplus_{k \in S}X_k \text{Tr}_{\mathcal{X}}[P_k(I_{\mathcal{X}} \otimes B(\mathcal{H}))P_k]X_k^\dagger \) is the null operator, one has

(63) \[ \oplus_{k \in S}B(\text{Rng}(X_k)) = \oplus_{k \in S}X_k \text{Tr}_{\mathcal{X}}[P_k(I_{\mathcal{X}} \otimes B(\mathcal{H}))P_k]X_k^\dagger. \]

\[ \mathbf{Corollary 6.} \quad \text{As in Theorem } 2, \text{ a necessary condition for extremality is } \]

(64) \[ \sum_{k \in S} \text{rank}(X_k)^2 \leq \dim(\mathcal{H})^2, \]

\[ \mathbf{Corollary 7.} \quad \text{Any rank-one covariant QO is extremal.} \]

\[ \mathbf{Proof.} \quad \text{For } \text{rank}(X) = 1 \text{ the set } S \text{ must contain only one equivalence class, and the iff condition } 17 \text{ of Theorem } 4 \text{ is then trivially satisfied.} \]

\[ \mathbf{Corollary 8.} \quad \text{For an irreducible representation any extremal covariant QO must be rank-one.} \]

\[ \mathbf{Corollary 9 (Choi).} \quad \text{In the non covariant case, a QO } \mathcal{M} \text{ from } B(\mathcal{H}) \text{ to } B(\mathcal{H}) \text{ is extremal iff it can be written in the form } \mathcal{M}(O) = \sum_i W_i^\dagger OW_i, \text{ with } W_i \in B(\mathcal{H}, \mathcal{X}) \text{ and the set of operators } \{W_i^\dagger W_j\} \text{ linearly independent.} \]

\[ \mathbf{Proof.} \quad \text{The non covariant case corresponds to the trivial covariance group } G = 1, \]

\[ \text{i. e. the group containing only the identity element. This corresponds to have just a single equivalence class, with multiplicity equal to } \dim(\mathcal{H} \otimes \mathcal{X}). \text{ Then, as in the proof of point } 2, \text{ of Theorem } 4 \text{ the extremality of } R = X^\dagger X \in B(\mathcal{H} \otimes \mathcal{X}) \text{ is equivalent to the injectivity of the map } \mathcal{M}(A) = \text{Tr}_{\mathcal{X}}[X^\dagger AX] \text{ on } B(\text{Rng}(X)). \]

According to Lemma 2 \( \text{using the singular value decomposition } X = \sum_i |V_i\rangle\langle W_i|, \)

\[ \text{with } |V_i\rangle \text{ orthonormal basis for } \text{Rng}(X) \text{ and } |W_i\rangle \in \mathcal{X} \otimes \mathcal{H}, \text{ one has } \mathcal{M}(O) = \sum_i W_i^\dagger OW_i \text{ for } O \in B(\mathcal{H}), \text{ and } \mathcal{M}(A) = \sum_{ij} (V_i \langle V_i| A W_j^\dagger W_j^\dagger) \text{ for } A \in B(\text{Rng}(X)), \)

and injectivity of \( \mathcal{M} \) is equivalent to linear independence of the set of operators \( \{W_i^\dagger W_j\} \). \]

Corollary 4 is the same as Choi theorem 17. Notice that differently from the case of QO’s, for POVM’s the non covariant case cannot be recovered as a special case of the covariant classification, since the group itself (or, more generally, the homogeneous factor space) coincides with the probability space \( \mathcal{X} \) of the POVM, whence trivializing \( G \) also trivializes \( \mathcal{X} \).
6.1. Example. Consider the phase-covariant cloning\cite{10,22} for equatorial qubits from 1 to 2 copies. This correspond to $G = \mathbb{U}(1)$, with representations $U_\phi = e^{i\phi}\ket{1}\bra{1}$ and $V_\phi = e^{i\phi}\sum_{s=0}^{1}\ket{1}\bra{1}$, where $s = 0$ denotes the input qubit and $s = 1, 2$ the output ones. Here $\mathcal{H} = \mathbb{C}^2$ and $\mathcal{K} = \mathcal{H} \otimes \mathcal{H}$. We first need to decompose the representation $V_\phi \otimes U_\phi^*$. This is made of one-dimensional representations, with characters $e^{ik\phi}$, with $k = -1, 0, 1, 2$ and multiplicities $m_{-1} = 1$, $m_0 = 3$, $m_1 = 3$, and $m_2 = 1$. The necessary condition (64) in the present case becomes $\sum_{k \in \mathbb{S}} \text{rank}(X_k)^2 \leq \dim(\mathcal{H}) = 4$, which means that we can have either a single equivalence class with $\text{rank}(X_k) = 2$, or two equivalence classes with $\text{rank}(X_k) = 1$ each. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k} \equiv \mathbb{C}^{m_k}$ of the $k$th equivalence class of irreducible representations are reported in Table 1 as subset of an orthonormal basis for the tensor product $\mathcal{H} \otimes \mathcal{H}$.

| $k$ | $|k_1\rangle \otimes |h_2\rangle$ |
|-----|-----------------------------|
| -1  | 001                         |
| 0   | 010, 011, 000               |
| 1   | 100, 101, 111               |
| 2   | 110                         |

Table 1. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k} \equiv \mathbb{C}^{m_k}$ of the $k$th equivalence class of irreducible representations for 1 to 2 phase-covariant cloning. The orthonormal basis are chosen as subsets of an orthonormal basis for the tensor product $\mathcal{H} \otimes \mathcal{H}$.

\[
\begin{array}{cccc}
S \triangleq \{k\} & \{\psi^{(k)}\} & \{\psi^{(k')}\} \\
\{\,-1,\,2\,\} & 001 & 110 \\
\{0,\,1\} & a|000\rangle + b|011\rangle + c|101\rangle & a'|111\rangle + b'|100\rangle + c'|010\rangle & |a|^2 + |b|^2 + |c|^2 = 1, \ |a'|^2 + |b'|^2 + |c'|^2 = 1 \\
\{0,\,-1\} & |000\rangle + a|011\rangle + b|101\rangle & c|001\rangle & |a|^2 + |b|^2 + |c|^2 = 1 \\
\{1,\,-1\} & a|100\rangle + b|010\rangle + c|111\rangle & d|001\rangle & |a|^2 + |b|^2 = 1, \ |c|^2 + \ |d|^2 = 1 \\
\{1,\,2\} & a|100\rangle + b|010\rangle + |111\rangle & d|110\rangle & |a|^2 + |b|^2 + |d|^2 = 1 \\
\{0,\,2\} & a|000\rangle + b|011\rangle + c|101\rangle & d|110\rangle & |a|^2 + |b|^2 + |d|^2 = 1 \\
\{0\} & \frac{1}{\sqrt{2}}|101\rangle + \frac{1}{\sqrt{2}}|011\rangle, |000\rangle \\
\{1\} & \frac{1}{\sqrt{2}}|010\rangle + \frac{1}{\sqrt{2}}|100\rangle, |111\rangle \\
\end{array}
\]

Table 2. Cloning from 1 to 2 copies: classification of operators $R = \sum_{k \in S} R_k = \sum_i |\psi^{(k)}_i\rangle \langle \psi^{(k)}_i|$ satisfying the necessary condition. 

The operators $R = \sum_{k \in S} R_k = \sum_i |\psi^{(k)}_i\rangle \langle \psi^{(k)}_i|$ satisfying the necessary conditions and the trace-preserving condition are reported in Table 2. It is easy to check that the case of $\text{rank}(X_k) = 2$ which would be possible only for $k = 0$ or $k = 1$
from 1 to 3 copies. This corresponds to (66).

As a specific optimization problem, let’s consider the maximization of the fidelity averaged over the two outputs

$$ F = \frac{1}{2} \left\{ \text{Tr}[\mathcal{M}^\dagger(\langle \psi \rangle |\psi\rangle)] + \text{Tr}[\mathcal{M}^\dagger(\langle \psi \rangle |\psi\rangle)] |\psi\rangle \right\} $$

and for equatorial qubits we can choose $|\psi\rangle = |\pm\rangle$, where $|\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle)$. Then the fidelity rewrites as

$$ F = \text{Tr}[WR_{\mathcal{M}}], $$

(67) $W = |\pm\rangle\langle \pm| \otimes |\pm\rangle\langle \pm| + \frac{1}{2} (|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|).$

One can see that $W$ is invariant under permutations over the output copies, and, by construction, also all vectors in Table 2 have the same symmetry. Due to the special form of the fidelity, the optimal map (satisfying $\mathcal{M}(I_{\mathcal{M}}) = I_{\mathcal{M}}$) is obtained for $S = \{0, 1\}$ with corresponding rank-two operator $R_{\mathcal{M}}$ given by

$$ R_{\mathcal{M}} = |\psi^{(0)}\rangle\langle \psi^{(0)}| + |\psi^{(1)}\rangle\langle \psi^{(1)}|, $$

$$ |\psi^{(0)}\rangle = \frac{1}{\sqrt{2}} (|000\rangle + \frac{1}{\sqrt{2}} |011\rangle + \frac{1}{\sqrt{2}} |100\rangle + |111\rangle), $$

$$ |\psi^{(1)}\rangle = \frac{1}{\sqrt{2}} (|111\rangle + \frac{1}{\sqrt{2}} |100\rangle + \frac{1}{\sqrt{2}} |011\rangle). $$

6.2. Example. Consider the phase-covariant cloning [16, 22] for equatorial qubits from 1 to 3 copies. This corresponds to $G = U(1)$, with representations $U_{\phi} = e^{i\phi |1\rangle\langle 1|}$ and $V_{\phi} = e^{i\phi \sum_{s=1}^{3} |1\rangle\langle 1|}$ where $s = 0$ denotes the input qubit and $s = 1, 2, 3$ the output ones. Here $\mathcal{H} = \mathbb{C}^2$ and $\mathcal{K} = \mathcal{K}^\otimes 3$. We first need to decompose the representation $V_{\phi} \otimes U_{\phi}^*$. This is made of one-dimensional representations, with characters $e^{ik\phi}$, with $k = -1, 0, 1, 2, 3$ and multiplicities $m_{-1} = 1, m_0 = 4, m_1 = 6, m_2 = 4$, and $m_3 = 1$. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k}$ of the $k$th equivalence class of irreducible representations for $S = 1$ to $3$ phase-covariant cloning. The orthonormal basis are chosen as subsets of an orthonormal basis for the tensor product $\mathcal{K} \otimes \mathcal{K}$.

| $k$ | $|k_i\rangle \otimes |h_j\rangle$ |
|-----|----------------------------------|
| -1  | [0001]                           |
| 0   | [1001], [0101], [0011], [0000]   |
| 1   | [1000], [0100], [0010], [1101], [1011], [0111] |
| 2   | [1100], [1010], [0110], [1111]   |
| 3   | [1110]                           |

Table 3. Orthonormal bases for the supporting spaces $\mathcal{H}_k \otimes \mathbb{C}^{m_k}$ of the $k$th equivalence class of irreducible representations for $S = 1$ to $3$ phase-covariant cloning. The orthonormal basis are chosen as subsets of an orthonormal basis for the tensor product $\mathcal{K} \otimes \mathcal{K}$. Again, since $\dim(\mathcal{H}) = 2$, the necessary condition (64) says that we can have only one equivalence class $k$ with $\text{rank}(X_k) \leq 2$, or two equivalence classes both with $\text{rank}(X_k) = 1$. In Ref. [22] it is shown that the map which optimizes the
averaged equatorial fidelity is actually given by the rank-one map for $S = \{1\}$ with 
corresponding operator $R_H$ given by

$$R_H = |\psi(1)\rangle \langle \psi(1)|, \tag{69}$$

$$|\psi(1)\rangle = \frac{1}{\sqrt{3}}(|1000\rangle + |0100\rangle + |0010\rangle + |1101\rangle + |1011\rangle + |0111\rangle).$$

Notice that, as a consequence of the specific symmetric form of the chosen fidelity 
criterion, the cloning maps of the examples $6.1$ and $6.2$ are both symmetrical, 
namely the output Hilbert space is indeed restricted to the symmetric tensor space 
$(\mathcal{H}^\otimes n)_\Sigma$. Clearly, with the same method also nonsymmetric types of cloning can 
be analyzed well.

6.3. Example. Consider a generic covariant QO with $\mathcal{H} \simeq \mathcal{H}$, $V_q = U_q$ and 
$G = SU(d)$, where $d = \text{dim}(\mathcal{H})$. In this case the representation $U_q \otimes U_q^*$ has 
two irreducible components: one which is one-dimensional, corresponding to the 
irreducible vector $|I\rangle \in \mathcal{H}^\otimes 2$, and one on the orthogonal complement, and the two 
components will be denoted by $k = 0$ and $k = 1$, respectively. Since both the 
irreducible components of the representation have unit multiplicity, the operator $R = X^\dagger X$ must have $X = \sum_{k \in S} c_k P_k$, $c_k \in \mathbb{C}$, $P_k$ denoting the orthogonal projector 
on the invariant space of the irreducible component $k$, and the necessary condition 
$|\psi(1)\rangle$ is trivially satisfied. On the other hand, one can see that the iff 
criterion $6.6$ is satisfied for the irreducible representations $S = \{0\}$ and $S = \{1\}$, whereas 
for the reducible one $S = \{0,1\}$ the map $\mathcal{F}(O) = \text{Tr}_\mathcal{H}[X^\dagger OX]$ is never injective 
on $\mathcal{A}_G \cap B(\text{Rng}(X))$ (one has $\text{Tr}_\mathcal{H}[X^\dagger OX] = \frac{1}{4}|\{c_0\}^2 a_0 + (d^2 - 1)|c_1|^2 a_1]|I\rangle\langle I|$ for 
$O = a_0 P_0 + a_1 P_1$, $a_0, a_1 \in \mathbb{C}$). Therefore, the only trace-preserving optimal maps 
are those corresponding to the operators $R = |I\rangle\langle I|$ and $R = \frac{d}{d^2-1}(|I^\otimes 2 - \frac{1}{d}|I\rangle\langle I|)$, 
corresponding to the trivial map $\mathcal{M} = \mathcal{I}$ and to the so-called isotropic depolarizing channel $\mathcal{M}(O) = \frac{d}{d^2-1}\text{Tr}(O)|I\rangle\langle I|$ $- \frac{1}{d^2-1}\rho$. Finally, notice that in the present 
example the optimal covariant maps are compatible only with (multiple of) the 
trace-preserving condition, since both partial traces $\text{Tr}_\mathcal{H}[P_k]$ are proportional to 
the identity.

6.4. Example. We consider now the same problem as in the previous example, 
but now with $V_q = U_q^*$. In this case we need to consider the positive operators $R$ 
which are invariant under $U_q^* \otimes U_q^*$. It will be easier to consider the representation 
$U_q \otimes U_q$ and then take the complex conjugate of $R$ at the end. Now we have again two 
irreducible inequivalent components, say $k = \pm$ with invariant spaces $(\mathcal{H}^\otimes 2)_{\pm}$, the 
symmetric and the antisymmetric spaces. As in the previous example, the general 
form of $R = X^\dagger X$ is $X = \sum_{k \in S} c_k P_k$, $c_k \in \mathbb{C}$, and $P_{\pm} = \frac{d}{d^2-1}(I_{\mathcal{H}} \pm E)$, where $E$ is 
the swap operator on the tensor product. However, the map $\mathcal{F}(O) = \text{Tr}_\mathcal{H}[X^\dagger OX]$ 
is injective on $\mathcal{A}_G \cap B(\text{Rng}(X))$ only for representations with a single irreducible 
component. One can see that $\text{Tr}_\mathcal{H}[P_{\pm}] = \frac{d}{d^2-1}(I_{\mathcal{H}} \pm E)$, and only trace-preserving 
(or multiplying by a constant) QO’s are compatible with the present covariance. 
In conclusion, the only extremal covariant operators are $R_{\pm} = (d \pm 1)^{-1}(I_{\mathcal{H}} \pm E)$, 
corresponding to the channels $\mathcal{M}_{\pm}(O) = (d \pm 1)^{-1}[\text{Tr}(O)I_{\mathcal{H}} \pm O^*]$. The map $\mathcal{M}_+$ 
is the optimal transposition map of Ref. [26].
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