Cones of positive maps and their duality relations

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The structure of cones of positive and k-positive maps acting on a finite-dimensional Hilbert space is investigated. Special emphasis is given to their duality relations to the sets of superpositive and k-superpositive maps. We characterize k-positive and k-superpositive maps with regard to their properties under taking compositions. A number of results obtained for maps are also rephrased for the corresponding cones of block positive, k-block positive, separable and k-entangled operators, due to the Jamiołkowski-Choi isomorphism. Generalizations to a situation where no such simple isomorphism is available are also made, employing the idea of mapping cones. As a side result to our discussion, we show that extreme entanglement witnesses, which are optimal, should be of special interest in entanglement studies.

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I. INTRODUCTION

Positive linear maps of C^*-algebras has been a subject of the mathematical literature for several years. In short, such a map sends the cone of positive operators acting from a given Hilbert space into itself. Note that we use the term "operators" when we refer to linear mappings of a general Hilbert space, but we only speak of "maps" when the elements of the underlying Hilbert space are already interpreted as operators.

A map Φ is called *k-positive* for some $k \in \mathbb{N}$ if the tensor product $\Phi \otimes \mathbb{1}_k$ is positive. When Φ is k-positive for any $k \in \mathbb{N}$, we call it *completely positive* (CP). The structure of the set of completely positive maps, which forms a proper subset of the set of positive maps, is already well understood. Due to the theorem of Stinespring [1], any CP map can be represented as a sum of *congruence maps*: $\mathrm{Ad}_{a_i} : x \mapsto a_i^* x a_i$, where * denotes the Hermitian conjugation, and the operators a_i are arbitrary. In physics literature the operators a_i are called *Kraus operators* [2], and it is possible to find such representation for which the number of them does not exceed d^2, where d is the dimension of the underlying Hilbert space $\mathcal{H}_d$. In general the operators a_i are of rank $\leqslant d$. In this paper we consider, among other classes, linear maps for which there exists a representation into Kraus operators of rank not greater than k, where $k = 1, \ldots, d-1$. These will be called *k-superpositive*, since in the case $k = 1$, the set of maps (denoted by $S(H)$ in [3]) for which all Kraus operators can be chosen to be of rank 1, coincides with the set of *superpositive maps*, introduced by Ando [4] (see also [5]). In the case when an additional trace-preserving condition is imposed, superpositive maps are often called *entanglement breaking channels* after the work by Horodecki, Shor and Ruskai [6].

Any linear map acting on the set $B(\mathcal{H}_d)$ of linear operators on $\mathcal{H}_d$ corresponds to an operator acting on the tensor product of Hilbert spaces $\mathcal{H}_d \otimes \mathcal{H}_d$. This fact, known as the *Jamiołkowski isomorphism* due to his early contribution [7], implies an intrinsic relation between the sets of quantum maps and quantum states [8, 9]. In particular, k-positive maps correspond to *k-block positive* operators [10, 11], which are positive on vectors of Schmidt rank $\leqslant k$. Accordingly, completely positive maps of $B(\mathcal{H}_d)$ correspond to positive operators on $\mathcal{H}_d \otimes \mathcal{H}_d$ [12]. A positive matrix representing a completely positive map in this isomorphism is called a *Choi matrix* or *dynamical matrix* [13]. It also turns out that k-superpositive maps are dual to *k-entangled* operators, which are convex combinations of projections onto vectors with Schmidt number not greater than k. Note that using this terminology, we could call separable operators 1-entangled, but we prefer to use the common name.

As we explain later, the sets of maps which are k-positive, completely positive and k-superpositive $(k = 1, \ldots, d-1)$ form a nested chain of proper subsets, see Table I and Fig. 1. Moreover, there exists a geometrical duality relation that links k-positive maps to k-superpositive maps for any $k = 1, \ldots, d-1$. By the Jamiołkowki-Choi isomorphism,

the same inclusion and duality relations hold for the corresponding sets of k-block positive, positive and k-entangled operators. We discuss this subject in more detail in Sections II and III. Table I summarizes on the mentioned dualities and on the notation we are going to use in what follows.

	Linear maps of $B(\mathcal{H}_d)$ $\mathcal{L}(\mathcal{H}_d)$		Operators acting on $\mathcal{H}_d \otimes \mathcal{H}_d$ $B(\mathcal{H}_d \otimes \mathcal{H}_d)$	
k	a) cone	b) dual cone	a') cone	b') dual cone
1	positive $\mathcal{P}(\mathcal{H}_d)$	superpositive $\mathcal{SP}(\mathcal{H}_d)$	block positive $BP(\mathcal{H}_d \otimes \mathcal{H}_d)$	separable $Sep(\mathcal{H}_d \otimes \mathcal{H}_d)$
2	2-positive $\mathcal{P}_2(\mathcal{H}_d)$	2-superpositive $\mathcal{SP}_2(\mathcal{H}_d)$	2-block positive $2\text{-}BP(\mathcal{H}_d \otimes \mathcal{H}_d)$	2-entangled $2\text{-}Ent(\mathcal{H}_d \otimes \mathcal{H}_d)$
...	...	...	...	...
$d-1$	$(d-1)$-positive $\mathcal{P}_{d-1}(\mathcal{H}_d)$	$(d-1)$-superpositive $\mathcal{SP}_{d-1}(\mathcal{H}_d)$	$(d-1)$-block positive $(d-1)\text{-}BP(\mathcal{H}_d \otimes \mathcal{H}_d)$	$(d-1)$-entangled $(d-1)\text{-}Ent(\mathcal{H}_d \otimes \mathcal{H}_d)$
d	completely positive $\mathcal{CP}(\mathcal{H}_d)$		positive $B^+(\mathcal{H}_d \otimes \mathcal{H}_d)$	

TABLE I: The cones of linear maps acting on the set of operators on $\mathcal{H}_d$ and the isomorphic cones of operators. Strict inclusion relations hold upwards ($\cup$) for the cones in columns a), a') and downwards ($\cap$) for the corresponding dual cones in columns b) and b'). Note that for $k = d$ the cones of d-positive and d-superpositive maps are both equal to the cone of completely positive maps. The same holds for the corresponding families of d-block positive, d-entangled and positive operators on $\mathcal{H}_d \otimes \mathcal{H}_d$. The cone of completely positive maps is selfdual and so is the corresponding cone of positive operators.

In spite of a considerable effort several years ago [3, 7, 10, 27–37] and more recently [38–47] the structure of the set of positive maps acting on operators defined on a d-dimensional Hilbert space $\mathcal{H}_d$ is well understood only for $d = 2$. In this case every positive map is decomposable, as it can be represented as a sum of a completely positive map and a completely co-positive map. This mathematical fact, following from the results of Størmer [27] and Woronowicz [32], has profound consequences for the entire theory of quantum entanglement. It implies that the commonly used PPT criterion for quantum separability [14] works in both directions for 2×2 quantum systems [15]. In other words, any state of a two qubit system is separable if and only if it has the property of positive partial transpose (PPT). Hence in this simplest case the sets of separable states and PPT states coincide, and any state characterized by a negative partial transpose is entangled.

This is not the case for higher dimensions. For instance, the existence of non-decomposable positive maps shown for $d = 3$ by Choi [31], implies that for a 3×3 quantum system there exist PPT entangled states. Such quantum states are called *bound entangled* [16], as they cannot be distilled into maximally entangled states, and their subtle properties became recently a subject of a vivid scientific interest [17, 18]. In general, the question of characterizing the set of entangled states for an arbitrary quantum system composed of two subsystems of size d, remains as one of the key unsolved problems in the theory of quantum information. However, from a mathematical perspective this problem is related to the characterization of the set of all positive maps in d dimensions, which is known to be difficult.

Since the set of block positive operators and separable operators are geometrically dual, any positive map (which is not completely positive) can be used to detect quantum entanglement. In particular, the Choi matrix representing such a map is given by a block positive operator and it may play the role of an *entanglement witness* [15, 19]. Such a Hermitian operator W is characterized by the property that $\mathrm{Tr}\,(W\sigma) \geqslant 0$ for any separable state σ, while negativity of $\mathrm{Tr}\,(W\rho)$ confirms that the analyzed state ρ is entangled. The key advantage of this notion is due to the fact that the Hermitian operator W can be considered as an observable, and the expectation value $\mathrm{Tr}\,(W\rho)$ can be decomposed into a sum of quantities which may be directly *measured* in a laboratory. In such a way one may experimentally confirm that an analyzed quantum state ρ is indeed entangled [20, 21]. Similar methods work for witnessing states of a given Schmidt number k [22, 23]. Then, k-block positive operators play the role of witnesses.

The set of entanglement witnesses thus corresponds to the set of block positive operators, the structure of which for $d \geqslant 3$ is still being investigated [24–26, 45]. It is worth to emphasize that there is no universal witness, which could detect entanglement of any state, but for any entangled state a suitable witness can be found. The most valuable are extreme entanglement witnesses, which form extreme points of the set of block positive operators, since they can also detect entanglement of some weakly entangled states. In this way the theory of quantum information provides a direct motivation to study the structure of the set of block positive operators (i.e. the set of entanglement witnesses) and its various subsets.

The aim of this work is to contribute to understanding of the non-trivial structure of the set of positive maps and the corresponding set of block positive operators. We provide a constructive characterization of various subsets of the set of positive maps. In particular we study relations based on duality between convex cones. Another class of results concerns composition of quantum maps.

This paper is organized as follows. In section 2 we review necessary definitions of k-positive and k-superpositive maps and formulate a kind of generalized Jamiołkowski-Choi theorem, which relates them to k-block positive and

k-entangled operators. Several other characterizations of these sets are proved. In section 3 we discuss the duality between the cones of k-positive and k-superpositive maps and analyze its consequences.

In section IV we study the relations of the results obtained in the previous sections to $\mathcal{K}$-positive maps, where $\mathcal{K}$ is a so-called *mapping cone*, introduced in [3].

II. CONES OF POSITIVE MAPS AND THE CORRESPONDING SETS OF OPERATORS

A. Maps of $B^+(\mathcal{H})$

In this section we give the definitions to which we refer in later parts of the paper and provide some concrete examples of objects that match these definitions. We review certain results already known in the literature and for convenience of the reader we prove some of them.

In the entire paper, we shall consider only finite dimensional linear spaces. Let $\mathcal{H} = \mathcal{H}_d$ be a Hilbert space of finite dimension d. We denote by $B(\mathcal{H})$ ($E(\mathcal{H})$, $B^+(\mathcal{H})$) the set of linear (resp. Hermitian, positive) operators on $\mathcal{H}$. We choose an orthonormal basis $\{e_i\}_{i=1}^d$ of $\mathcal{H}$ and the corresponding complete set of matrix units $\{e_{ij}\}_{i,j=1}^d$ in $B(\mathcal{H})$.

Let us consider the set $\mathcal{L}(\mathcal{H})$ of linear maps sending $B(\mathcal{H})$ into itself. An element Φ of $\mathcal{L}(\mathcal{H})$ is called *Hermiticity preserving* iff $\Phi(E(\mathcal{H})) \subset E(\mathcal{H})$. *Positive maps* are the elements Φ which fulfill $\Phi(B^+(\mathcal{H})) \subset B^+(\mathcal{H})$. The set of Hermiticity preserving maps will be denoted by $\mathcal{E}(\mathcal{H})$ and the set of positive maps by $\mathcal{P}(\mathcal{H})$. It is easy to show (cf. [50]) that positivity of $\Phi \in \mathcal{L}(\mathcal{H})$ implies the Hermiticity preserving property, so we have the inclusion $\mathcal{P}(\mathcal{H}) \subset \mathcal{E}(\mathcal{H})$. Let k be a positive integer. The family of *k-positive maps*, $\mathcal{P}_k(\mathcal{H})$, is defined by the condition $\mathbb{1}_k \otimes \Phi \in \mathcal{P}(\mathbb{C}^k \otimes \mathcal{H})$. That is, $\Phi \in \mathcal{L}(\mathcal{H})$ is k-positive iff the tensor product of Φ by the k-dimensional identity map $\mathbb{1}_k$ remains positive. A different characterization of k-positivity is given in the following lemma,

Lemma II.1. *Let Φ be an element of $\mathcal{L}(\mathcal{H})$. The map Φ is k-positive iff the map*

$$B(\mathcal{H} \otimes \mathcal{H}) \ni x \longmapsto (\mathbb{1}_d \otimes \Phi)(q \otimes \mathbb{1}_d) x (q \otimes \mathbb{1}_d) \in B(\mathcal{H} \otimes \mathcal{H}) \tag{1}$$

is positive for an arbitrary k-dimensional orthogonal projection q in $\mathcal{H}$.

Proof. Let $q = \sum_{i=1}^k |f_i\rangle \langle f_i|$, where $\{f_i\}_{i=1}^d$ is an orthonormal basis of $\mathcal{H}$. We choose $\{f_i \otimes e_j\}_{i,j=1}^d$ as the orthonormal basis of $\mathcal{H} \otimes \mathcal{H}$. The map (1) is positive iff it is positive on all one dimensional projections on $\mathcal{H} \otimes \mathcal{H}$,

$$(\mathbb{1}_d \otimes \Phi)(q \otimes \mathbb{1}_d) |\psi\rangle \langle \psi| (q \otimes \mathbb{1}_d) \geqslant 0 \, \forall_{\psi \in \mathcal{H} \otimes \mathcal{H}}. \tag{2}$$

This is the same as

$$\langle\phi|\left(\mathbb{1}_d\otimes\Phi\right)\left(q\otimes\mathbb{1}_d\right)|\psi\rangle\,\langle\psi|\left(q\otimes\mathbb{1}_d\right)\phi\rangle\geqslant 0\,\forall_{\psi,\phi\in\mathcal{H}\otimes\mathcal{H}}. \tag{3}$$

Let $\psi=\sum_{i,j=1}^d\psi^{ij}f_i\otimes e_j$ and $\phi=\sum_{i,j=1}^d\phi^{ij}f_i\otimes e_j$. Because of the assumed form of q, in index notation the condition (3) reads

$$\sum_{r,s=1}^d\sum_{j,m=1}^d\sum_{i,l=1}^k\left(\phi^{ir}\right)^*\Phi_{rs,jm}\psi^{ij}\left(\psi^{lm}\right)^*\phi^{ls}\geqslant 0 \tag{4}$$

for all $\left\{\psi^{ij}\right\}_{i,j=1}^{i=k,j=d},\left\{\phi^{lm}\right\}_{l,m=1}^{l=k,m=d}\subset\mathbb{C}$. Here $\Phi_{rs,jm}$ denote the matrix elements of Φ with respect to the standard basis of $B\left(\mathcal{H}\right)$, $\Phi\left(e_{jm}\right)=\sum_{r,s=1}^d\Phi_{rs,jm}e_{rs}$. But eq. (4) is the same as

$$\langle\phi|\left(\left(\mathbb{1}_k\otimes\Phi\right)|\psi\rangle\,\langle\psi|\right)\phi\rangle\geqslant 0\,\forall_{\psi,\phi\in\mathbb{C}^k\otimes\mathcal{H}}. \tag{5}$$

This condition means that $\left(\mathbb{1}_k\otimes\Phi\right)|\psi\rangle\,\langle\psi|\geqslant 0$ for any one-dimensional projector $|\psi\rangle\,\langle\psi|$ on $\mathbb{C}^k\otimes\mathcal{H}$, which is equivalent to k-positivity of Φ. $\qquad\square$

If Φ is k-positive for every $k\in\mathbb{N}$, we call it *completely positive*. We shall denote the family of completely positive maps with $\mathcal{CP}\left(\mathcal{H}\right)$. Obviously, $\mathcal{CP}\left(\mathcal{H}\right)=\bigcap_{k\in\mathbb{N}}\mathcal{P}_k\left(\mathcal{H}\right)$, but it is also a well known fact [12] that for $k\geqslant d$, we get $\mathcal{P}_k\left(\mathcal{H}\right)=\mathcal{CP}\left(\mathcal{H}\right)$. A natural question arises whether the sets $\mathcal{P}_k\left(\mathcal{H}\right)$ with $k\leqslant d$ are all distinct one from another. An affirmative answer can be found in [48]. For $k=1,\dots,d$, the map

$$\phi_\lambda:B\left(\mathcal{H}\right)\ni a\mapsto\operatorname{Tr}a\mathbb{1}_d-\frac{\lambda}{d}a \tag{6}$$

turns out to be k-positive iff $\lambda\geqslant\frac{1}{k}$. This is a generalization of the famous example by Choi [30] of a map that is $(d-1)$-positive, but not completely positive,

$$\phi_{Choi}:B\left(\mathcal{H}\right)\ni a\mapsto\operatorname{Tr}a\mathbb{1}_d-\frac{d}{d-1}a. \tag{7}$$

Consider an operator $a\in B\left(\mathcal{H}\right)$. It defines a *congruence map* (also called *conjugation by a*): $\operatorname{Ad}_a:B\left(\mathcal{H}\right)\ni x\mapsto a^*xa\in B\left(\mathcal{H}\right)$. For any operator a such a map is completely positive. As observed by Kraus [2], any completely positive map can be written in the form $\sum_{i=1}^n\operatorname{Ad}_{a_i}$ for some $\{a_i\}_{i=1}^n\subset B\left(\mathcal{H}\right)$ ($n\in\mathbb{N}$). The converse holds trivially, so we get $\mathcal{CP}\left(\mathcal{H}\right)=\operatorname{convhull}\{\operatorname{Ad}_a|a\in B\left(\mathcal{H}\right)\}$. If we impose additional conditions on the operators a_i, we get even stronger properties of $\Phi=\sum_{i=1}^n\operatorname{Ad}_{a_i}$ than complete positivity.

For $k\in\mathbb{N}$, we say that Φ is k-*superpositive* iff there exists a Kraus representation of Φ such that all the operators a_i are of rank not greater than k. We denote the set of k-superpositive maps by $\mathcal{SP}_k\left(\mathcal{H}\right)$. Obviously, $\mathcal{SP}_k\left(\mathcal{H}\right)=\mathcal{CP}\left(\mathcal{H}\right)$

for $k \geqslant d$. It is natural to ask whether the classes $\mathcal{SP}_k(\mathcal{H})$ with $k \leqslant d$ are all distinct one from another. It turns out that they are, as follows from the Proposition II.6 at the end of this section. Maps which are 1-superpositive are simply called *superpositive* [4] and we abbreviate the notation $\mathcal{SP}_1(\mathcal{H})$ to $\mathcal{SP}(\mathcal{H})$.

All the sets of operators that we introduced above have their corresponding left transposed partners. For any $\mathcal{A} \subset \mathcal{L}(\mathcal{H})$, we define

$$\mathcal{A}^\tau := \{t \circ \Phi | \Phi \in \mathcal{A}\}, \tag{8}$$

where t is the transpose map. It is customary that the name of $\mathcal{A}^\tau$ differs from the name of $\mathcal{A}$ by a "co" suffix. For example, $\mathcal{CP}(\mathcal{H})^\tau$ is called the set of *completely copositive* maps. One can easily check that $\mathcal{P}(\mathcal{H}) = \mathcal{P}(\mathcal{H})^\tau$ and $\mathcal{SP}(\mathcal{H}) = \mathcal{SP}(\mathcal{H})^\tau$.

As a conclusion of the above discussion, we get the following chain of inclusions

$$\mathcal{SP}(\mathcal{H}) \subset \mathcal{SP}_2(\mathcal{H}) \subset \ldots \subset \mathcal{SP}_{d-1}(\mathcal{H}) \subset \mathcal{CP}(\mathcal{H}) \subset \mathcal{P}_{d-1}(\mathcal{H}) \subset \ldots \subset \mathcal{P}_2(\mathcal{H}) \subset \mathcal{P}(\mathcal{H}), \tag{9}$$

where all the inclusions are strict, see Proposition II.6 (cf. also columns b) and a) in Table I).

Finally, we define the following three families of maps ($k, m \in \mathbb{N}$),

$$\mathcal{D}_{k,m}(\mathcal{H}) := \mathcal{P}_k(\mathcal{H}) \vee (\mathcal{P}_m(\mathcal{H}))^\tau, \tag{10}$$

$$\mathcal{P}_{k,m}(\mathcal{H}) := \mathcal{P}_k(\mathcal{H}) \cap (\mathcal{P}_m(\mathcal{H}))^\tau, \tag{11}$$

$$\mathcal{S}_{k,m}(\mathcal{H}) := \mathcal{SP}_k(\mathcal{H}) \cap (\mathcal{SP}_m(\mathcal{H}))^\tau. \tag{12}$$

We call them (k, m)-*decomposable*, (k, m)-*positive* and (k, m)-*superpositive* maps, respectively. Obviously, $\mathcal{P}_{k,0}(\mathcal{H}) = \mathcal{P}_k(\mathcal{H})$, $\mathcal{S}_{k,0}(\mathcal{H}) = \mathcal{SP}_k(\mathcal{H})$, $\mathcal{P}_{0,m}(\mathcal{H}) = (\mathcal{P}_m(\mathcal{H}))^\tau$ and $\mathcal{S}_{0,m}(\mathcal{H}) = (\mathcal{SP}_m(\mathcal{H}))^\tau$, so all the previously discussed classes of maps are included in the definitions (11) and (12). It is also easy to see that $\mathcal{D}_{k,m}(\mathcal{H})^\tau = \mathcal{D}_{m,k}(\mathcal{H})$, $\mathcal{P}_{k,m}(\mathcal{H})^\tau = \mathcal{P}_{m,k}(\mathcal{H})$ and $\mathcal{S}_{k,m}(\mathcal{H})^\tau = \mathcal{S}_{m,k}(\mathcal{H})$ in general. Note that similar families of maps and inclusion relations between them were analyzed by Chruściński and Kossakowski [45], who called k-superpositive maps *partially entanglement breaking channels*. In [49] the author defines a family of maps which he calls "2-decomposable", but they correspond to $\mathcal{S}_{0,2}(\mathcal{H})$ in our notation. That is, we call them "2-supercopositive maps". On the other hand, the families $\mathcal{D}_{2,2}(\mathbb{C}^3)$ and $\mathcal{D}_{2,2}(\mathbb{C}^4)$, which we would call 2-decomposable, appeared many times in the context of *atomic maps* [38, 56, 57]. An element of $\mathcal{L}(\mathcal{H})$ is called atomic iff it does not belong to $\mathcal{D}_{2,2}(\mathcal{H})$. In particular, in [38] it was proved that all the known generalized indecomposable Choi maps of $B(\mathbb{C}^3)$ are atomic. This falsifies the possible conjecture that the Størmer-Woronowicz theorem ([27], [32]) has a generalization of the form $\mathcal{P}(\mathbb{C}^n) = \mathcal{D}_{n-1,n-1}(\mathbb{C}^n)$.

B.   Operators on $\mathcal{H} \otimes \mathcal{H}$

Linear operators on $B(\mathcal{H})$ ("maps") can be identified with corresponding elements of $B(\mathcal{H} \otimes \mathcal{H})$ ("operators"). In the following, we shall introduce the $B(\mathcal{H} \otimes \mathcal{H})$ counterparts of the families of maps that we defined above.

Let Φ be an element of $\mathcal{L}(\mathcal{H})$. Following Jamiołkowski [7] and Choi [12], we define

$$C_\Phi := \sum_{i,j=1}^{d} e_{ij} \otimes \Phi(e_{ij}) = (\mathbb{1} \otimes \Phi) |\Psi_+\rangle \langle \Psi_+|, \tag{13}$$

where $\Psi_+ = \sum_i e_i \otimes e_i$ is a maximally entangled state on $\mathcal{H} \otimes \mathcal{H}$. We shall denote the map $\Phi \mapsto C_\Phi$ by J,

$$J : \mathcal{L}(\mathcal{H}) \ni \Phi \longmapsto (\mathbb{1} \otimes \Phi) |\Psi_+\rangle \langle \Psi_+| \in B(\mathcal{H} \otimes \mathcal{H}). \tag{14}$$

It is well known [7, 28] that $J|_{\mathcal{E}(\mathcal{H})}$ is an isomorphism between $\mathcal{E}(\mathcal{H})$ and the set of Hermitian operators on $\mathcal{H} \otimes \mathcal{H}$, $E(\mathcal{H} \otimes \mathcal{H})$. Since $\mathcal{P}(\mathcal{H}) \subset \mathcal{E}(\mathcal{H})$, we shall concentrate on $\Phi|_{\mathcal{E}(\mathcal{H})}$ in most of what follows and we omit the subscript $|_{\mathcal{E}(\mathcal{H})}$. Thus J can be regarded as a $\mathbb{R}$-linear isomorphism between the $\mathbb{R}$-linear spaces $\mathcal{E}(\mathcal{H})$ and $E(\mathcal{H} \otimes \mathcal{H})$.

Let us introduce the so-called set of k-block positive operators $(k \in \mathbb{N})$,

$$k\text{-}BP(\mathcal{H} \otimes \mathcal{H}) := \left\{ a \left| \left\langle \sum_{i=1}^{k} \phi_i \otimes \psi_i \middle| a \sum_{l=1}^{k} \phi_l \otimes \psi_l \right\rangle \geqslant 0 \, \forall_{\{\psi_i\}_{i=1}^{k}, \{\phi_i\}_{l=1}^{k} \subset \mathcal{H}} \right. \right\}, \tag{15}$$

where the a's are elements of $B(\mathcal{H} \otimes \mathcal{H})$. We write $BP(\mathcal{H} \otimes \mathcal{H})$ instead of 1-$BP(\mathcal{H} \otimes \mathcal{H})$ and simply call 1-block positive operators *block positive*. One can easily prove that $k\text{-}BP(\mathcal{H} \otimes \mathcal{H}) \subset E(\mathcal{H} \otimes \mathcal{H})$ for arbitrary $k \geqslant 1$ (cf. [50]). Moreover, we have the following

Proposition II.2. (Generalized Jamiołkowski-Choi theorem) *Let k be a positive integer. The sets $\mathcal{P}_k(\mathcal{H})$ and $k\text{-}BP(\mathcal{H} \otimes \mathcal{H})$ are isomorphic. We have*

$$J(\mathcal{P}_k(\mathcal{H})) = k\text{-}BP(\mathcal{H} \otimes \mathcal{H}), \tag{16}$$

where the isomorphism J was defined in (14).

Proof. Let Φ be an element of $\mathcal{E}(\mathcal{H})$. We shall prove that $\Phi \in \mathcal{P}_k(\mathcal{H})$ is equivalent to $C_\Phi \in k\text{-}BP(\mathcal{H} \otimes \mathcal{H})$ and thus we will have proved (16). We start from the following lemma,

Lemma II.3. *Let $\Phi \in \mathcal{E}(\mathcal{H})$ and denote by $\Phi_{ij,kl}$ the matrix elements of Φ with respect to the standard basis of $B(\mathcal{H})$, $\Phi(e_{kl}) = \sum_{i,j=1}^{d} \Phi_{ij,kl} e_{ij}$. Let $C_\Phi = (C_\Phi)_{rs,tu} e_{rt} \otimes e_{su}$, so that $(C_\Phi)_{rs,tu}$ are the coefficients of C_Φ with respect to the basis $\{e_{rt} \otimes e_{su}\}_{r,t,s,u=1}^{d}$. Then we have*

$$(C_\Phi)_{ij,kl} = \Phi_{jl,ik}. \tag{17}$$

Proof. By definition (see (13)), $C_\Phi = \sum_{r,s=1}^d e_{rs} \otimes \Phi(e_{rs})$. In index notation,

$$(C_\Phi)_{ij,kl} = \sum_{r,s=1}^d (e_{rs} \otimes \Phi(e_{rs}))_{ij,kl} = \sum_{r,s=1}^d (e_{rs})_{ik} (\Phi(e_{rs}))_{jl}. \tag{18}$$

From (18) we readily get

$$(C_\Phi)_{ij,kl} = \sum_{r,s=1}^d \delta_{ri}\delta_{sk} (\Phi(e_{rs}))_{jl} = \sum_{r,s=1}^d \delta_{ri}\delta_{sk} \Phi_{jl,rs} = \Phi_{jl,ik}, \tag{19}$$

which is the expected formula. Such a reordering of elements of the superoperator Φ, first used by Sudarshan et al. [13] to obtain the matrix C_Φ, was later called *reshuffling* [51]. $\qquad\square$

Now we can prove Proposition II.2. When applied to C_Φ, the k-block positivity condition that appears in (15) may be rewritten in index notation as

$$\sum_{r,s=1}^d \sum_{j,m=1}^d \sum_{i,l=1}^k (\psi_i^r)^* \phi_i^j (C_\Phi)_{rj,sm} (\phi_l^m)^* \psi_l^s \geqslant 0 \tag{20}$$

for all $\left\{\psi_i^j\right\}_{i,j=1}^{i=k,j=d}$, $\{\phi_l^m\}_{l,m=1}^{l=k,m=d} \subset \mathbb{C}$. Since this should hold for arbitrary sets of complex numbers ψ_i^j, ϕ_l^m, we can complex conjugate all of them in (20). We also change the names of indices like $j \leftrightarrow r$ and $m \leftrightarrow s$. After all these changes we get as equivalent to (20),

$$\sum_{r,s=1}^d \sum_{j,m=1}^d \sum_{i,l=1}^k \psi_i^j (\phi_i^r)^* (C_\Phi)_{jr,ms} \phi_l^s (\psi_l^m)^* \geqslant 0, \tag{21}$$

which should hold for all $\left\{\psi_i^j\right\}_{i,j=1}^{i=k,j=d}$, $\{\phi_l^m\}_{l,m=1}^{l=k,m=d} \subset \mathbb{C}$.

Using Lemma II.3, we may rewrite (21) as

$$\sum_{r,s=1}^d \sum_{j,m=1}^d \sum_{i,l=1}^k (\psi_i^r)^* \phi_i^j \Phi_{rs,jm} (\phi_l^m)^* \psi_l^s \geqslant 0. \tag{22}$$

After small rearrangements, this is precisely condition (4). The only difference is that the position of the first index in ϕ^{ij} and in ψ^{lm} was changed, which is not significant. As we mentioned in the proof of Lemma II.1, (4) is equivalent to k-positivity of Φ and so is (22). $\qquad\square$

Proposition II.2 appears in the early work by Takasaki and Tomiyama, [10] (it was also proved in [11] using different methods). Thus we have found the $B(\mathcal{H} \otimes \mathcal{H})$ counterparts of the sets $\mathcal{P}_k(\mathcal{H})$. In particular, the case $k = 1$ gives the relation between positive maps and block positive operators, analyzed by Jamiołkowski [7]. On the other hand, for any $k \geqslant d$ one has that k-$BP(\mathcal{H} \otimes \mathcal{H}) = B^+(\mathcal{H} \otimes \mathcal{H})$. A similar equality holds between $\mathcal{P}_k(\mathcal{H})$ and $\mathcal{CP}(\mathcal{H})$ for $k \geqslant d$. Using Proposition II.2, we recover the Choi's well known result [12],

Proposition II.4 (Choi)**.** *The set of completely positive maps of $B(\mathcal{H})$ is isomorphic to the set of positive operators on composed Hilbert space,*

$$J\left(\mathcal{CP}\left(\mathcal{H}\right)\right) = B^+\left(\mathcal{H}\otimes\mathcal{H}\right). \tag{23}$$

$\square$

Thus for intermediate integer values, $k = 2,\ldots,d-1$, we get a kind of discrete interpolation between the theorems of Jamiołkowski and Choi.

To find the sets of operators corresponding to k-superpositive maps, we shall need the following lemma,

Lemma II.5. *Let $a \in B(\mathcal{H})$. Then*

$$C_{\mathrm{Ad}_a} = |\alpha\rangle\langle\alpha|, \tag{24}$$

where $\alpha \in \mathcal{H}\otimes\mathcal{H}$, $r := \mathrm{rk}\,a$ (rk denotes the rank of a) and

$$\alpha = \sum_{l=1}^{r} \phi_l \otimes \psi_l \tag{25}$$

for some orthogonal vectors $\{\phi_i\}_{i=1}^r, \{\psi_j\}_{j=1}^r \subset \mathcal{H}$. Any operator $|\alpha\rangle\langle\alpha|$ with α of the form (25) can be obtained as C_{Ad_a} for some $a \in B(\mathcal{H})$.

Proof. From the polar decomposition of a, we have $a = \sum_{l=1}^r \sqrt{\lambda_l} U |\psi_l\rangle\langle\psi_l|$, where the λ_l's are the eigenvalues of $|a| := \sqrt{a^*a}$, U is a unitary operator on $\mathcal{H}$ and the vectors $\psi_l \in \mathcal{H}$ are orthonormal. By the definition (13),

$$C_{\mathrm{Ad}a} = \sum_{l,m=1}^{r}\sum_{i,j=1}^{d} e_{ij} \otimes \sqrt{\lambda_l\lambda_m}\,\langle\psi_l|\,U^*e_{ij}U\psi_m\rangle\,|\psi_l\rangle\langle\psi_m| \tag{26}$$

Define $\tilde{\psi}_l = \sqrt{\lambda_l}\sum_{i=1}^d\sum_{j=1}^d U_j^i \psi_l^j e_i$ and $\phi_l = \sqrt{\lambda_l}\sum_{i=1}^d \left(\sum_{j=1}^d U_j^i\psi_l^j\right)^* e_i$, where $\psi_l = \sum_{j=1}^d \psi_l^j e_j$ and U_j^i are matrix elements of U. The vectors ϕ_i are mutually orthogonal. We get

$$C_{\mathrm{Ad}a} = \sum_{l,m=1}^{r}\sum_{i,j=1}^{d} \left\langle \tilde{\psi}_l \middle| e_{ij}\tilde{\psi}_m \right\rangle e_{ij} \otimes |\psi_l\rangle\langle\psi_m| \tag{27}$$

It is easy to show that $\sum_{i,j=1}^d \left\langle \tilde{\psi}_l \middle| e_{ij}\tilde{\psi}_m \right\rangle e_{ij} = |\phi_l\rangle\langle\phi_m|$. Hence (27) can be rewritten as

$$C_{\mathrm{Ad}a} = \sum_{l,m=1}^{r} |\phi_l\rangle\langle\phi_m| \otimes |\psi_l\rangle\langle\psi_m|, \tag{28}$$

which equals $|\alpha\rangle\langle\alpha|$ for $\alpha = \sum_{l=1}^r \phi_l \otimes \psi_l$. This proves the main part of the lemma. The fact that any projector $|\alpha\rangle\langle\alpha|$ can be obtained in this way follows from the calculation of C_{Ad_a} for $a = \sum_{i=1}^k |\tilde{\phi}_i\rangle\langle\psi_i|$. $\square$

Using Lemma II.5, we can prove the promised result that all the sets $\mathcal{P}_k(\mathcal{H})$ for $k = 1, \ldots, \mathcal{H}$ are distinct. We have the following

Proposition II.6. *Let $k \leqslant d$ be a positive integer. Let $a \in B(\mathcal{H})$ and $\operatorname{rk} a = k$. The congruence map Ad_a is an element of $\mathcal{SP}_k(\mathcal{H})$, but not of $\mathcal{SP}_{k-1}(\mathcal{H})$.*

Proof. Let a be as in the assumptions of the proposition. Obviously, Ad_a is an element of $\mathcal{SP}_k(\mathcal{H})$. Let us assume $\operatorname{Ad}_a = \sum_i \operatorname{Ad}_{a_i}$ for some nonzero operators $\{a_i\}_{i=1}^m \subset B(\mathcal{H})$. By calculating the Choi matrices of both sides of this equality, we get from Lemma II.5

$$|\alpha\rangle\langle\alpha| = \sum_{l=1}^m |\alpha_l\rangle\langle\alpha_l| \tag{29}$$

for some $m \in \mathbb{N}$ and nonzero vectors $\alpha \in \mathcal{H}$, $\{\alpha_l\}_{l=1}^m \subset \mathcal{H}$ such that $C_a = |\alpha\rangle\langle\alpha|$ and $C_{a_l} = |\alpha_l\rangle\langle\alpha_l|$. But (29) can only hold if all the vectors α_l are scalar multiples of α. According to Lemma II.5, α is of the form $\sum_{l=1}^k \phi_l \otimes \psi_l$, so all the vectors α_l have to be of the same form as well. Using Lemma II.5 again, we conclude that $\operatorname{rk} a_l = k$. Since we made no assumptions about the a_l's, the equality $\operatorname{rk} a_l = k$ implies that Ad_a cannot be an element of $\mathcal{SP}_{k-1}(\mathcal{H})$. This proves our assertion [60]. $\qquad\square$

In short, Proposition II.6 implies that the inclusion $\mathcal{SP}_{k-1}(\mathcal{H}) \subset \mathcal{SP}_k(\mathcal{H})$ is strict for $k \leqslant d$, as we already mentioned above.

Lemma II.5 can as well be used to find the families of operators in $B(\mathcal{H} \otimes \mathcal{H})$ corresponding to k-superpositive maps. By the very definition of $\mathcal{SP}_k(\mathcal{H})$, an element $\Phi \in \mathcal{L}(\mathcal{H})$ is k-superpositive iff it is of the form $\sum_{l=1}^m \operatorname{Ad}_{a_l}$ for some $m \in \mathbb{N}$ and $\{a_l\}_{l=1}^m \subset B(\mathcal{H})$ such that $\operatorname{rk} a_l \leqslant k$ for all $l = 1, \ldots, m$. According to Lemma II.5, this is the same as

$$C_\Phi = \sum_{i,j=1}^k \sum_{l=1}^m \left|\phi_i^{(l)} \otimes \psi_i^{(l)}\right\rangle \left\langle \phi_j^{(l)} \otimes \psi_j^{(l)}\right| \tag{30}$$

for some $m \in \mathbb{N}$ and sets of vectors $\left\{\phi_i^{(l)}\right\}_{i=1}^k, \left\{\psi_j^{(l)}\right\}_{j=1}^k \in \mathcal{H}$, where $l = 1, \ldots, m$. We do not assume the vectors to be nonzero. Obviously, operators on the right hand side of (30) make up the convex cone spanned by the positive rank 1 operators $\sum_{i,j=1}^k |\phi_i \otimes \psi_i\rangle\langle\phi_j \otimes \psi_j|$. This is nothing else as the definition of an operator with the *Schmidt number* equal to k - see [11, 53, 55].

Thus we get the following

Proposition II.7. *Let k be a positive integer. Let us define the set of k-entangled operators on $\mathcal{H} \otimes \mathcal{H}$ (equivalent to the set of operators with Schmidt number less than or equal to k),*

$$k\text{-}Ent\left(\mathcal{H} \otimes \mathcal{H}\right) := \text{convhull}\left\{\sum_{i,j=1}^{k} |\phi_i \otimes \psi_i\rangle \langle\phi_j \otimes \psi_j| \,\middle|\, \{\phi_i\}_{i=1}^{k}, \{\psi_j\}_{j=1}^{k} \subset \mathcal{H}\right\}. \tag{31}$$

Thus the set of k-superpositive maps is isomorphic to $k\text{-}Ent\left(\mathcal{H} \otimes \mathcal{H}\right)$,

$$J\left(\mathcal{SP}_k\left(\mathcal{H}\right)\right) = k\text{-}Ent\left(\mathcal{H} \otimes \mathcal{H}\right). \tag{32}$$

$\square$

We can now write a chain of inclusions corresponding to (9),

$$Sep \subset \ldots \subset (d-1)\text{-}Ent \subset B^+ \subset (d-1)\text{-}BP \subset \ldots \subset BP, \tag{33}$$

where all the the inclusions are strict (we omit the brackets $(\mathcal{H} \otimes \mathcal{H})$ to fit the formula into the page and write Sep instead of $1\text{-}Ent$ to simplify notation. The elements of $Sep\left(\mathcal{H} \otimes \mathcal{H}\right)$ are called *separable* operators). This chain of inclusions, studied earlier in [45], corresponds to columns b') and a') in Table I on page 3.

To find the sets of operators corresponding to completely copositive $(\mathcal{CP}\left(\mathcal{H}\right)^\tau)$, k-copositive $(\mathcal{P}_k\left(\mathcal{H}\right)^\tau)$ and k-supercopositive maps $(\mathcal{SP}_k\left(\mathcal{H}\right)^\tau)$, we use the following lemma

Lemma II.8. *Let $\mathcal{A}$ be a subset of $\mathcal{L}\left(\mathcal{H}\right)$ and $J\left(\mathcal{A}\right) \subset B\left(\mathcal{H} \otimes \mathcal{H}\right)$. We have*

$$J\left(\mathcal{A}^\tau\right) = \left(\mathbb{1} \otimes t\right) J\left(\mathcal{A}\right) := \left\{\left(\mathbb{1} \otimes t\right) a \,\middle|\, a \in J\left(\mathcal{A}\right)\right\}, \tag{34}$$

Proof. From the definition (13), we have

$$C_{t\circ\Phi} = \left(\mathbb{1} \otimes \left(t \circ \Phi\right)\right) |\Psi_+\rangle \langle\Psi_+| = \left(\mathbb{1} \otimes t\right)\left(\mathbb{1} \otimes \Phi\right) |\Psi_+\rangle \langle\Psi_+| = \left(\mathbb{1} \otimes t\right) C_\Phi. \tag{35}$$

This gives us $J\left(t \circ \Phi\right) = \left(\mathbb{1} \otimes t\right) J\left(\Phi\right)$, which proves the lemma. $\square$

The map $\mathbb{1} \otimes t$ that appears in Lemma II.8 is called *partial transposition*. Using the lemma, we trivially get

Proposition II.9. *Let k be a positive integer. We have the correspondences*

$$J\left(\mathcal{CP}\left(\mathcal{H}\right)^\tau\right) = \left(\mathbb{1} \otimes t\right) B^+\left(\mathcal{H} \otimes \mathcal{H}\right), \tag{36}$$

$$J\left(\mathcal{P}_k\left(\mathcal{H}\right)^\tau\right) = \left(\mathbb{1} \otimes t\right) k\text{-}BP\left(\mathcal{H} \otimes \mathcal{H}\right), \tag{37}$$

$$J\left(\mathcal{SP}_k\left(\mathcal{H}\right)^\tau\right) = \left(\mathbb{1} \otimes t\right) k\text{-}Ent\left(\mathcal{H} \otimes \mathcal{H}\right). \tag{38}$$

$\square$

The sets $\mathcal{D}_{k,m}(\mathcal{H})$, $\mathcal{P}_{k,m}(\mathcal{H})$ and $\mathcal{S}_{k,m}(\mathcal{H})$ also have their $B(\mathcal{H} \otimes \mathcal{H})$ counterparts,

Proposition II.10. *Let k, m be positive integers. We have*

$$J(\mathcal{D}_{k,m}(\mathcal{H})) = k\text{-}BP(\mathcal{H} \otimes \mathcal{H}) \vee (\mathbb{1} \otimes t) \, m\text{-}BP(\mathcal{H} \otimes \mathcal{H}), \tag{39}$$

$$J(\mathcal{P}_{k,m}(\mathcal{H})) = k\text{-}BP(\mathcal{H} \otimes \mathcal{H}) \cap (\mathbb{1} \otimes t) \, m\text{-}BP(\mathcal{H} \otimes \mathcal{H}), \tag{40}$$

$$J(\mathcal{S}_{k,m}(\mathcal{H})) = k\text{-}Ent(\mathcal{H} \otimes \mathcal{H}) \cap (\mathbb{1} \otimes t) \, m\text{-}Ent(\mathcal{H} \otimes \mathcal{H}). \tag{41}$$

$\square$

III. RELATIONS BETWEEN k-POSITIVE AND k-SUPERPOSITIVE MAPS. OTHER RELATIONS

It is a well known fact that $E(\mathcal{H} \otimes \mathcal{H})$ is a d^4-dimensional vector space over $\mathbb{R}$ and it is equipped with the symmetric *Hilbert-Schmidt product*,

$$a \cdot b := \mathrm{Tr}(a^* b) = \mathrm{Tr}(ab), \tag{42}$$

where $a, b \in E(\mathcal{H} \otimes \mathcal{H})$, and the last equality holds due to the Hermiticity of a.

Let A be a cone in $E(\mathcal{H} \otimes \mathcal{H})$. We define the *dual cone* of A,

$$A^\circ := \{b \in E(\mathcal{H} \otimes \mathcal{H}) | \, a \cdot b \geqslant 0 \, \forall_{a \in A}\}. \tag{43}$$

By comparing the definitions (15) and (31), we easily get

Proposition III.1. $k\text{-}BP(\mathcal{H} \otimes \mathcal{H}) = (k\text{-}Ent(\mathcal{H} \otimes \mathcal{H}))^\circ$

Proof. Follows directly from the definition of $k\text{-}BP(\mathcal{H} \otimes \mathcal{H})$ if we observe that

$$\left\langle \sum_{i=1}^{k} \phi_i \otimes \psi_i \middle| a \sum_{j=1}^{k} \phi_j \otimes \psi_j \right\rangle = \mathrm{Tr}\left(a \sum_{i,j=1} |\phi_j \otimes \psi_j\rangle \langle \phi_i \otimes \psi_i| \right). \tag{44}$$

$\square$

By substituting $k = d$, we get $(B^+(\mathcal{H} \otimes \mathcal{H}))^\circ = B^+(\mathcal{H} \otimes \mathcal{H})$, which was discussed in [8, 45], and may easily be proved directly. Remember that we have $d\text{-}Ent(\mathcal{H} \otimes \mathcal{H}) = d\text{-}BP(\mathcal{H} \otimes \mathcal{H}) = B^+(\mathcal{H} \otimes \mathcal{H})$.

From the existence of separating hyperplanes in $\mathbb{R}^n$ (cf. Theorem 14.1 in [54]) it follows that $(A^\circ)^\circ = \bar{A}$ for any cone $A \in E(\mathcal{H} \otimes \mathcal{H})$. In particular,

$$(A^\circ)^\circ = A \tag{45}$$

for a closed convex cone $A \subset E(\mathcal{H} \otimes \mathcal{H})$. We call this fact the *bidual theorem*. As a consequence, we have

Proposition III.2. $k\text{-}Ent\left(\mathcal{H}\otimes\mathcal{H}\right)=\left(k\text{-}BP\left(\mathcal{H}\otimes\mathcal{H}\right)\right)^{\circ}$

Proof. In is easy to show that the set $k\text{-}Ent\left(\mathcal{H}\otimes\mathcal{H}\right)$ is closed (cf. e.g. [50]). Thus we can use the bidual theorem together with Proposition III.1 to prove our assertion. $\qquad\square$

Using the natural duality in $E\left(\mathcal{H}\otimes\mathcal{H}\right)$, we can introduce an analogous operation in $\mathcal{E}\left(\mathcal{H}\right)$. Let $\mathcal{X}\subset\mathcal{E}\left(\mathcal{H}\right)$ be a convex cone. We define the *dual cone* of $\mathcal{X}$ as

$$\mathcal{X}^{\circ}:=\left\{\Phi\in\mathcal{E}\left(\mathcal{H}\right)\middle|\operatorname{Tr}\left(C_{\Phi}C_{\Psi}\right)\geqslant 0\,\forall_{\Psi\in\mathcal{X}}\right\}. \tag{46}$$

It is easy to notice that (46) can as well be written as

$$\left(\mathcal{X}\right)^{\circ}=J^{-1}\left(\left(J\left(\mathcal{X}\right)\right)^{\circ}\right), \tag{47}$$

which makes the definition (46) transparent. As a direct consequence of (47) and Propositions II.2 and III.1, we obtain

Proposition III.3. $\mathcal{P}_{k}\left(\mathcal{H}\right)=\mathcal{SP}_{k}\left(\mathcal{H}\right)^{\circ}$ $\qquad\square$

In a similar way, using Propositions II.7 and III.2, we obtain

Proposition III.4. $\mathcal{SP}_{k}\left(\mathcal{H}\right)=\mathcal{P}_{k}\left(\mathcal{H}\right)^{\circ}$ $\qquad\square$

This result was given in a slightly less explicit way in [39].

Remembering that $\mathcal{SP}_{d}\left(\mathcal{H}\right)=\mathcal{P}_{d}\left(\mathcal{H}\right)=\mathcal{CP}\left(\mathcal{H}\right)$, we easily obtain from Proposition III.3 or III.4 the relation $\mathcal{CP}\left(\mathcal{H}\right)^{\circ}=\mathcal{CP}\left(\mathcal{H}\right)$. *The set of completely positive maps is self-dual.*

Using the results presented above, it is straightforward to show the following

Corollary III.5. *Let k,m be positive integers. We have $\mathcal{D}_{k,m}\left(\mathcal{H}\right)^{\circ}=\mathcal{S}_{k,m}\left(\mathcal{H}\right)$ and $\mathcal{S}_{k,m}\left(\mathcal{H}\right)^{\circ}=\mathcal{D}_{k,m}\left(\mathcal{H}\right)$* $\qquad\square$

The next result, related to composition properties of maps [45, 50, 51], will be crucial for our later discussion

Theorem III.6. $\mathcal{SP}_{k}\left(\mathcal{H}\right)\circ\mathcal{P}_{k}\left(\mathcal{H}\right)=\mathcal{P}_{k}\left(\mathcal{H}\right)\circ\mathcal{SP}_{k}\left(\mathcal{H}\right)=\mathcal{SP}_{k}\left(\mathcal{H}\right)$

Proof. Being more explicit, we want to prove that $\Phi\circ\Psi\in\mathcal{SP}_{k}\left(\mathcal{H}\right)$ and $\Psi\circ\Phi\in\mathcal{SP}_{k}\left(\mathcal{H}\right)$ for arbitrary $k\in\mathbb{N}$, whenever $\Phi\in\mathcal{SP}_{k}\left(\mathcal{H}\right)$ and $\Psi\in\mathcal{P}_{k}\left(\mathcal{H}\right)$. It is sufficient to show this for $\Phi=\operatorname{Ad}_{a}$ with an arbitrary $a\in B\left(\mathcal{H}\right)$ of rank $\leqslant k$. We prove first that $\Psi\circ\operatorname{Ad}_{a}$ is an element of $\mathcal{SP}_{k}\left(\mathcal{H}\right)$. For this we shall need the following lemma

Lemma III.7. *Let $\Psi \in \mathcal{L}(\mathcal{H})$ be k-positive. For any k-element set of vectors $\{\psi_i\}_{i=1}^k$, there exists $m \in \mathbb{N}$ and vectors $\left\{\xi_l^{(n)}\right\}_{l,n=1}^{l=k,n=m}$ such that*

$$\Psi\left(|\psi_i\rangle\langle\psi_j|\right) = \sum_{n=1}^m \left|\xi_i^{(n)}\right\rangle\left\langle\xi_j^{(n)}\right| \tag{48}$$

for all $i, j \in \{1, \ldots, k\}$.

Proof. The operator $\left[\Psi\left(|\psi_i\rangle\langle\psi_j|\right)\right]_{i,j=1}^k$ belongs to $B\left(\mathbb{C}^k \otimes \mathcal{H}\right)$. Since ψ is positive, $\left[\Psi\left(|\psi_i\rangle\langle\psi_j|\right)\right] \in B^+\left(\mathbb{C} \otimes \mathcal{H}\right)$, hence is a sum of positive rank 1 operators, which are necessarily of the form $\left[\left|\xi_i^{(n)}\right\rangle\left\langle\xi_j^{(n)}\right|\right]_{i,j=1}^k$ with $\left\{\xi_l^{(n)}\right\}_{l,n=1}^{l=k,n=m}$ as in the statement of the theorem. $\square$

Now we can prove that $\Psi \circ \mathrm{Ad}_a \in \mathcal{SP}_k(\mathcal{H})$. Let us take an arbitrary element $x \in B(\mathcal{H})$. The fact that $\mathrm{rk}\, a \leqslant k$ is equivalent to $a = \sum_{i=1}^k |\phi_i\rangle\langle\psi_i|$ for some vectors $\{\phi_i\}_{i=1}^k, \{\psi_j\}_{j=1}^k \subset \mathcal{H}$. Thus we get

$$\mathrm{Ad}_a(x) = \sum_{i,j=1}^k \langle\phi_i|\, x\phi_j\rangle\, |\psi_i\rangle\langle\psi_j|. \tag{49}$$

Now we calculate the action of $\Psi \circ \mathrm{Ad}_a$ on x,

$$(\Psi \circ \mathrm{Ad}_a)\, x = \sum_{i,j=1}^k \langle\phi_i|\, x\phi_j\rangle\, \Psi\left(|\psi_i\rangle\langle\psi_j|\right) = \sum_{l=1}^m \sum_{i,j=1}^k \langle\phi_i|\, x\phi_j\rangle \left|\xi_i^{(l)}\right\rangle\left\langle\xi_j^{(l)}\right|. \tag{50}$$

This is a sum of terms of the form (49) and we get $\Psi \circ \mathrm{Ad}_a = \sum_{l=1}^m \mathrm{Ad}_{a_l}$, where the operators $a_l := \sum_{j=1}^k |\phi_j\rangle\langle\xi_j^{(l)}|$ all have rank lower or equal k. Thus we have proved $\Psi \circ \mathrm{Ad}_a \in \mathcal{SP}_k(\mathcal{H})$, which implies that $\Psi \circ \Phi \in \mathcal{SP}_k(\mathcal{H})$ for arbitrary $\Phi \in \mathcal{SP}_k(\mathcal{H})$. We still need to show that $\Phi \circ \Psi \in \mathcal{SP}_k(\mathcal{H})$. This can be easily deduced from the following lemma,

Lemma III.8. *Let Φ be an element of $\mathcal{SP}_k(\mathcal{H})$ and Ψ an element of $\mathcal{P}_k(\mathcal{H})$. Let Φ^*, Ψ^* be the adjoint operators of Φ, Ψ (resp.) with respect to the Hilbert-Schmidt product on $B(\mathcal{H})$, given by the formula (42) with $a, b \in B(\mathcal{H})$. We have $\Phi^* \in \mathcal{SP}_k(\mathcal{H})$ and $\Psi^* \in \mathcal{P}_k(\mathcal{H})$.*

Proof. Just as $B^+(\mathcal{H} \otimes \mathcal{H})$, the set $B^+\left(\mathbb{C}^k \otimes \mathcal{H}\right)$ is self-dual. Thus we have that $x \in B^+\left(\mathbb{C}^k \otimes \mathcal{H}\right) \Leftrightarrow \mathrm{Tr}(x^*y) \geqslant 0\, \forall_{y \in B^+(\mathbb{C}^k \otimes \mathcal{H})}$. The definition of k-positivity of Ψ can be restated as

$$\mathrm{Tr}\left(\left(\left(\mathbb{1}_k \otimes \Psi\right)x\right)^* y\right) \geqslant 0\, \forall_{x,y \in B^+(\mathbb{C}^k \otimes \mathcal{H})}. \tag{51}$$

Equivalently,

$$\mathrm{Tr}\left(\left(\left(\mathbb{1}_k \otimes \Psi^*\right)y\right)^* x\right) \geqslant 0\, \forall_{x,y \in B^+(\mathbb{C}^k \otimes \mathcal{H})}. \tag{52}$$

But this is just the condition (51) for Ψ^*. Hence $\Psi \in \mathcal{P}_k(\mathcal{H}) \Leftrightarrow \Psi^* \in \mathcal{P}_k(\mathcal{H})$. To prove an analogous equivalence for Φ, it is enough to consider the specific case $\Phi = \mathrm{Ad}_a$ with $\mathrm{rk}\, a \leqslant k$. We have

$$\mathrm{Tr}\left((\mathrm{Ad}_a(x))^* y\right) = \mathrm{Tr}\left((a^* x a)^* y\right) = \mathrm{Tr}\left(x^* (a y a^*)^*\right) = \mathrm{Tr}\left(x \left(\mathrm{Ad}_{a^*}(y)\right)^*\right) \tag{53}$$

This gives us $(\mathrm{Ad}_a)^* = \mathrm{Ad}_{a^*}$. The ranks of a and a^* are equal, so $\mathrm{Ad}_a \in \mathcal{SP}_k(\mathcal{H}) \Leftrightarrow (\mathrm{Ad}_a)^* \in \mathcal{SP}_k(\mathcal{H})$, which implies $\Phi \in \mathcal{SP}_k(\mathcal{H}) \Leftrightarrow \Phi^* \in \mathcal{SP}_k(\mathcal{H})$ and finishes the proof of the lemma. $\qquad\square$

Now we can finish the proof of Theorem III.6. By Lemma III.8, $\Phi \circ \Psi \in \mathcal{SP}_k(\mathcal{H})$ is equivalent to $(\Phi \circ \Psi)^* = \Psi^* \circ \Phi^* \in \mathcal{SP}_k(\mathcal{H})$. The last equality holds according to Lemma III.8 and to the first part of the theorem. $\qquad\square$

In short, we proved that for any Φ k-superpositive and Ψ k-positive, the products $\Phi \circ \Psi$ and $\Psi \circ \Phi$ are k-superpositive.

It is good to notice that Theorem III.6 justifies the name *entanglement breaking channels*, which is often used for superpositive, trace preserving maps of $B(\mathcal{H})$. To make this precise, we show the following

Corollary III.9. *Let Φ be superpositive. For any $\rho \in B^+(\mathcal{H} \otimes \mathcal{H})$, we have*

$$(\mathbb{1} \otimes \Phi)\rho \in Sep(\mathcal{H} \otimes \mathcal{H}) \tag{54}$$

Proof. Since $J(\mathcal{CP}(\mathcal{H})) = B^+(\mathcal{H} \otimes \mathcal{H})$, where J is the isomorphism defined in (14), we have

$$\rho = (\mathbb{1} \otimes \Psi)\ket{\psi_+}\bra{\psi_+} \tag{55}$$

for a suitably chosen $\Psi \in \mathcal{CP}(\mathcal{H})$. We have

$$(\mathbb{1} \otimes \Phi)\rho = (\mathbb{1} \otimes \Phi)(\mathbb{1} \otimes \Psi)\ket{\psi_+}\bra{\psi_+} = (\mathbb{1} \otimes \Phi \circ \Psi)\ket{\psi_+}\bra{\psi_+}. \tag{56}$$

Because $\mathcal{CP}(\mathcal{H})$ is a subset of $\mathcal{P}(\mathcal{H})$, Ψ is an element of $\mathcal{P}(\mathcal{H})$ an we get from Theorem III.6 the inclusion $\Phi \circ \Psi \in \mathcal{SP}(\mathcal{H})$. By Proposition II.7, the operator $(\mathbb{1} \otimes \Phi \circ \Psi)\ket{\psi_+}\bra{\psi_+}$ is separable. Comparing this with (56), we immediately see that (54) is true. $\qquad\square$

Obviously, it is possible to repeat the argument given above in the case when we assume k-superpositivity of Φ and demand k-separability of $(\mathbb{1} \otimes \Phi)\rho$. Therefore one could think of calling k-superpositive and trace preserving maps *k-separability inducing channels*.

We shall finish this section with a number of characterizations of the sets $\mathcal{SP}_k(\mathcal{H})$ and $\mathcal{P}_k(\mathcal{H})$. Together with Theorem III.6, the following four theorems should be regarded as some of the most important material included in the paper and be studied with care.

Theorem III.10. *Let $\Phi \in \mathcal{E}(\mathcal{H})$ and $k \in \mathbb{N}$. The following conditions are equivalent:*

1) $\Phi \in \mathcal{SP}_k(\mathcal{H})$,

2) $\Psi \circ \Phi \in \mathcal{SP}_k(\mathcal{H}) \; \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$,

3) $\Psi \circ \Phi \in \mathcal{CP}(\mathcal{H}) \; \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$,

4) $\mathrm{Tr}\left(|\psi_+\rangle\langle\psi_+|\left(\mathbb{1} \otimes (\Psi \circ \Phi)\right)(|\psi_+\rangle\langle\psi_+|)\right) \geqslant 0 \; \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$.

Proof. 1) $\Rightarrow$ 2) As we know from Theorem III.6, $\Psi \circ \Phi \in \mathcal{SP}_k(\mathcal{H})$ for $\Psi \in \mathcal{P}_k(\mathcal{H})$ and $\Phi \in \mathcal{SP}_k(\mathcal{H})$. This proves 2)

2) $\Rightarrow$ 3) This implication is obvious because $\mathcal{SP}_k(\mathcal{H}) \subset \mathcal{P}_k(\mathcal{H})$

3) $\Rightarrow$ 4) We know from 3) that $\Psi \circ \Phi$ is completely positive. As a consequence of Choi's theorem (Proposition II.4), $C_{\Psi \circ \Phi} = (\mathbb{1} \otimes (\Psi \circ \Phi))(|\psi_+\rangle\langle\psi_+|)$ is positive. Thus we have $\mathrm{Tr}\left(|\psi_+\rangle\langle\psi_+| C_{\Psi \circ \Phi}\right) \geqslant 0$, which is precisely the statement in 4).

4) $\Rightarrow$ 1) Let $\Theta_{\Psi,\Phi}$ denote $\mathrm{Tr}\left(|\psi_+\rangle\langle\psi_+|\left(\mathbb{1} \otimes (\Psi \circ \Phi)\right)(|\psi_+\rangle\langle\psi_+|)\right)$. We calculate

$$
\begin{aligned}
\Theta_{\Psi,\Phi} &= \mathrm{Tr}\left(|\psi_+\rangle\langle\psi_+|\,(\mathbb{1} \otimes \Psi) \circ (\mathbb{1} \otimes \Phi)(|\psi_+\rangle\langle\psi_+|)\right) &= \\
&= \mathrm{Tr}\left((\mathbb{1} \otimes \Psi)^* (|\psi_+\rangle\langle\psi_+|)(\mathbb{1} \otimes \Phi)(|\psi_+\rangle\langle\psi_+|)\right) &= \\
&= \mathrm{Tr}\left((\mathbb{1} \otimes \Psi^*)(|\psi_+\rangle\langle\psi_+|)(\mathbb{1} \otimes \Phi)(|\psi_+\rangle\langle\psi_+|)\right) &= \mathrm{Tr}\left(C_{\Psi^*} C_\Phi\right).
\end{aligned}
\tag{57}
$$

Thus the condition $\Theta_{\Psi,\Phi} \geqslant 0 \; \forall_{\Psi \in \mathcal{P}_\mathcal{H}}$, which we have in 4), is the same as

$$
\mathrm{Tr}\left(C_{\Psi^*} C_\Phi\right) \geqslant 0 \; \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}
\tag{58}
$$

Using Lemma III.8 again, we see that (58) is equivalent to

$$
\mathrm{Tr}\left(C_\Psi C_\Phi\right) \geqslant 0 \; \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}.
\tag{59}
$$

Comparing this with the definition (46) of the dual cone of $\mathcal{P}_k(\mathcal{H})$ and using Proposition III.4, we obtain

$$
\Phi \in \left(\mathcal{P}_k(\mathcal{H})\right)^\circ = \mathcal{SP}_k(\mathcal{H}),
\tag{60}
$$

which is 1). $\qquad\square$

The following three characterization theorems can be proved in practically the same way as Theorem III.10.

Theorem III.11. *Let $\Phi \in \mathcal{E}(\mathcal{H})$ and $k \in \mathbb{N}$. The following conditions are equivalent:*

1) $\Phi \in \mathcal{SP}_k(\mathcal{H})$,

2) $\Phi \circ \Psi \in \mathcal{SP}_k (\mathcal{H}) \ \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$,

3) $\Phi \circ \Psi \in \mathcal{CP} (\mathcal{H}) \ \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$,

4) $\mathrm{Tr} \left(|\psi_+\rangle \langle\psi_+| \left(\mathbb{1} \otimes (\Phi \circ \Psi) \right) \left(|\psi_+\rangle \langle\psi_+| \right) \right) \geqslant 0 \ \forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$.

$\square$

Theorem III.12. *Let $\Phi \in \mathcal{E} (\mathcal{H})$ and $k \in \mathbb{N}$. The following conditions are equivalent:*

1) $\Phi \in \mathcal{P}_k (\mathcal{H})$,

2) $\Psi \circ \Phi \in \mathcal{SP}_k (\mathcal{H}) \ \forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$,

3) $\Psi \circ \Phi \in \mathcal{CP} (\mathcal{H}) \ \forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$,

4) $\mathrm{Tr} \left(|\psi_+\rangle \langle\psi_+| \left(\mathbb{1} \otimes (\Psi \circ \Phi) \right) \left(|\psi_+\rangle \langle\psi_+| \right) \right) \geqslant 0 \ \forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$.

$\square$

Theorem III.13. *Let $\Phi \in \mathcal{E} (\mathcal{H})$ and $k \in \mathbb{N}$. The following conditions are equivalent:*

1) $\Phi \in \mathcal{P}_k (\mathcal{H})$,

2) $\Phi \circ \Psi \in \mathcal{SP}_k (\mathcal{H}) \ \forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$,

3) $\Phi \circ \Psi \in \mathcal{CP} (\mathcal{H}) \ \forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$,

4) $\mathrm{Tr} \left(|\psi_+\rangle \langle\psi_+| \left(\mathbb{1} \otimes (\Phi \circ \Psi) \right) \left(|\psi_+\rangle \langle\psi_+| \right) \right) \geqslant 0 \ \forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$.

$\square$

Theorem III.11 is much the same as Theorem III.10, but the order of the operators Ψ, Φ is different in these theorems. Theorems III.12 and III.13 are in complete analogy with III.10 and III.11 (resp.), but the roles of k-positive and k-superpositive maps have been exchanged. In section 4 we shall add two more to the list of equivalent conditions in the the above theorems, see Corollaries IV.3 and IV.4.

We should remark that the four theorems given above make up a broad generalization of a number of relatively well known facts about the sets $\mathcal{P} (\mathcal{H})$, $\mathcal{CP} (\mathcal{H})$ and $\mathcal{SP} (\mathcal{H})$,

$$\Phi \in \mathcal{SP} (\mathcal{H}) \iff \Psi \circ \Phi \in \mathcal{CP} (\mathcal{H}) \ \forall_{\Psi \in \mathcal{P}(\mathcal{H})} \tag{61}$$

$$\Phi \in \mathcal{CP} (\mathcal{H}) \iff \Psi \circ \Phi \in \mathcal{CP} (\mathcal{H}) \ \forall_{\Psi \in \mathcal{CP}(\mathcal{H})} \tag{62}$$

$$\Phi \in \mathcal{P} (\mathcal{H}) \iff \Psi \circ \Phi \in \mathcal{CP} (\mathcal{H}) \ \forall_{\Psi \in \mathcal{SP}(\mathcal{H})} \tag{63}$$
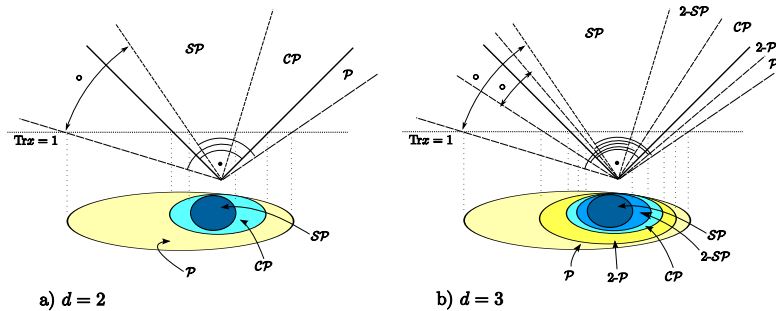
Figure 1: Cones of positive maps: a) $d = 2$, self-dual cone $\mathcal{CP}(\mathcal{H}) = (\mathcal{CP}(\mathcal{H}))^\circ$ and a pair of dual cones $\mathcal{P}(\mathcal{H}) = \mathcal{SP}(\mathcal{H})^\circ$; b) case $d = 3$ with yet another pair of dual cones $\mathcal{P}_2(\mathcal{H}) = (\mathcal{SP}_2(\mathcal{H}))^\circ$. The plot above shows unbounded cones and the normalization hyperplane $\mathrm{Tr}\,x = 1$, while the convex sets below represent their cross-sections. The same sketch is applicable to the corresponding cones of block positive, positive semidefinite and separable operators.
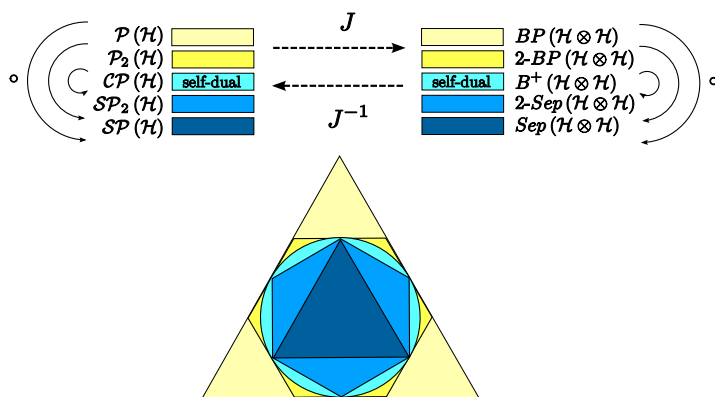
Figure 2: A schematic picture of the chain of inclusions $\mathcal{SP}(\mathcal{H}) \subsetneq \mathcal{SP}_2(\mathcal{H}) \subsetneq \mathcal{CP}(\mathcal{H}) \subsetneq \mathcal{P}_2(\mathcal{H}) \subsetneq \mathcal{P}(\mathcal{H})$ ($d \geqslant 3$), which takes into account the duality relations expressed in Propositions III.3 and III.4. The same sketch represents also the inclusion relations among the sets of normalized operators, which correspond to sets of maps with respect to the Jamiołkowski isomorphism J.

(these can be found on page 345 of [51]). We should emphasize that the results like (61)-(63) and our four theorems do not simply follow from the closedness relations of the type $\Phi, \Psi \in \mathcal{CP}(\mathcal{H}) \Rightarrow \Phi \circ \Psi \in \mathcal{CP}(\mathcal{H})$ (and similarly for $\mathcal{P}(\mathcal{H})$, $\mathcal{P}_k(\mathcal{H})$, $\mathcal{SP}_k(\mathcal{H})$ and $\mathcal{SP}(\mathcal{H})$).

A.   A geometry detour

We find it useful to explain the duality between the cones of maps using simple examples taken from three-dimensional Euclidean geometry. The relations expressed in Propositions III.3 and III.4 can be depicted as in Figure 1,

which shows the cones of block-positive, positive and separable operators for $d = 2$ and $d = 3$. Note that the self-dual cone for positive operators is represented by the right-angled triangle. The same sketch represents also the corresponding cones of maps. In physical application one is often interested in a set of normalized operators. For instance, the trace normalization $\operatorname{Tr} x = 1$ corresponds to a hyperplane, represented by a horizontal line.

The cross-section of such a normalization hyperplane with each cone gives bounded convex sets of a finite volume estimated in [59]. Their structure for $d = 3$ is sketched in Fig. 2. The picture is exact in the sense that there exist convex cones in $\mathbb{R}^3$ such that their section by an appropriately chosen plane gives the above sets which fulfill the duality relations in accordance with Propositions III.3 and III.4. For example, the circle in Figure 2 is a section of a cone of aperture $\pi/2$ by a plane perpendicular to its axis. The cone is self-dual, just as the set $\mathcal{CP}(\mathcal{H})$ which it represents.
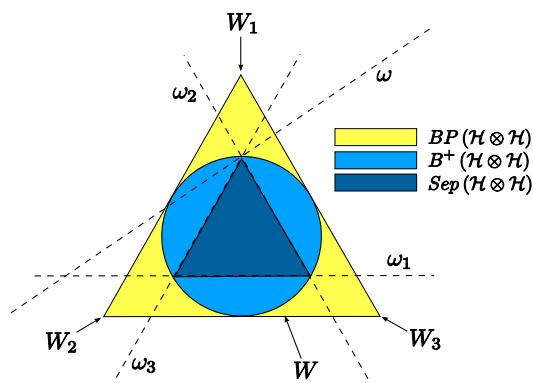

Figure 3: A sketch of the set of block positive operators (entanglement witnesses) for $d = 2$. It includes the set of positive operators (quantum states) and the set of separable states. Three optimal witnesses (W_1, W_2, W_3) are the extreme points of BP and the corresponding dual lines (ω_1, ω_2, ω_3) determine completely the shape of the set of separable states in this plot. No other element W of the border of $BP(\mathcal{H})$ is optimal (ω denotes the line dual to W).

By modifying Figure 2 a little, we get a sketch that illustrates the important notion of an *optimal entanglement witness* [24] (cf. also [52]). By definition, a block positive operator $W \in B(\mathcal{H} \otimes \mathcal{H})$ is called *optimal* if and only if the set $\Delta_W := \{\rho \in B^+(\mathcal{H}) \,|\, \operatorname{Tr}(\rho W) < 0\}$ is maximal (with respect of inclusion) within the family of sets $\Delta_{W'}$ (for $W' \in BP(\mathcal{H} \otimes \mathcal{H})$). It is known [24] that optimal witnesses have to lie on the boundary of $BP(\mathcal{H} \otimes \mathcal{H})$. In the case of Figure 3, optimal witnesses coincide with the extreme points of $BP(\mathcal{H} \otimes \mathcal{H})$. This is specific to the particular pictorial representation that we use. In reality, there exist optimal entanglement witnesses that are not extreme. Still, not every optimal witness is needed to determine the shape of the set of separable states, $Sep(\mathcal{H} \otimes \mathcal{H}) = BP(\mathcal{H} \otimes \mathcal{H})^\circ$. It is in principle possible to consider only the optimal witnesses which are extreme points of the intersection of $BP(\mathcal{H} \otimes \mathcal{H})$

with the hyperplane $\operatorname{Tr} W = 1$. This is so because we have the following propositions, [61]

Proposition III.14. *An operator* $\rho \in B\left(\mathcal{H} \otimes \mathcal{H}\right)$ *is separable iff* $\operatorname{Tr}\left(W \rho\right) \geqslant 0$ *for all* W *extreme in* $BP\left(\mathcal{H} \otimes \mathcal{H}\right)' :=$ $\left\{W \in BP\left(\mathcal{H} \otimes \mathcal{H}\right) \mid \operatorname{Tr} W = 1\right\}$.

Proof. The "only if" part is obvious from Proposition III.4. Let $\mathrm{e}BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$ denote the set of extreme points of $BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$. The "if" part of the proposition follows because $BP\left(\mathcal{H} \otimes \mathcal{H}\right)' = \operatorname{convhull} \mathrm{e}BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$ as well as $BP\left(\mathcal{H} \otimes \mathcal{H}\right) = \mathbb{R}_0^+ BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$, where the first equality is a consequence of the Krein-Milman theorem ($BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$ is compact) and the latter holds because a block positive operator W has zero trace only if $W = 0$. All in all, we get $BP\left(\mathcal{H} \otimes \mathcal{H}\right) = \mathbb{R}_0^+ \operatorname{convhull} \mathrm{e}BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$ and the proposition follows from Proposition III.4 by using the linearity of the trace. $\square$

Proposition III.15. *Every extreme point of* $BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$ *is an optimal entanglement witness.*

Proof. According to Theorem 1 in [24], an entanglement witness W is optimal iff $(1 + \varepsilon)W - \varepsilon P \notin BP\left(\mathcal{H} \otimes \mathcal{H}\right)$ for arbitrary $\varepsilon > 0$ and a nonzero $P \in B^+\left(\mathcal{H} \otimes \mathcal{H}\right)$. Assume that W is an extreme point in $BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$ and $(1 + \varepsilon)W - \varepsilon P \in BP\left(\mathcal{H} \otimes \mathcal{H}\right)$ for some $\varepsilon > 0$, $P \in B^+\left(\mathcal{H} \otimes \mathcal{H}\right) \setminus \{0\}$. This is the same as $W - \xi P \in BP\left(\mathcal{H} \otimes \mathcal{H}\right)$ for some $\xi > 0$ or $W - \upsilon P / \operatorname{Tr} P \in BP\left(\mathcal{H} \otimes \mathcal{H}\right)$ for some $\upsilon > 0$. Then, of course, $W' := (1 + \upsilon)W - \upsilon P / \operatorname{Tr} P$ is an element of $BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$. But this contradicts extremality of W since $W = W'/(1 + \upsilon) + \upsilon P /((1 + \upsilon) \operatorname{Tr} P)$, $1/(1 + \upsilon) + \upsilon/(1 + \upsilon) = 1$ and both W' and $P / \operatorname{Tr} P$ are elements of $BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$. Thus $(1 + \varepsilon)W - \varepsilon P \notin BP\left(\mathcal{H} \otimes \mathcal{H}\right)$ for arbitrary $\varepsilon > 0$ and $P \in B^+\left(\mathcal{H} \otimes \mathcal{H}\right) \setminus \{0\}$, so W is optimal. $\square$

It is therefore natural to define *extreme entanglement witnesses* as the extreme points of $BP\left(\mathcal{H} \otimes \mathcal{H}\right)'$ and to give priority to witnesses which are not only optimal, but also extreme. We have

$$\textbf{extreme entanglement witnesses} = \textbf{extreme points of } \mathbf{BP}\left(\mathcal{H} \otimes \mathcal{H}\right)',$$

and in principle, no other witnesses are needed to describe the set of separable states.

It should be kept in mind that Fig. 3 presents a highly simplified sketch of the problem. Even in the simplest possible case of a 2×2 system the set of separable states is 15 dimensional and it is well known that this convex set is not a polytope and its geometry is rather involved [51]. Nevertheless, a very clear characterization of optimal entanglement witnesses that does not substantially depend on the dimension has recently been obtained by G. Sarbicki [26].

IV. MAPPING CONES

In the previous sections we have studied maps of $B(\mathcal{H})$ into itself for $\mathcal{H}$ a finite dimensional Hilbert space, and much of the technical work has involved the Choi matrix (13) and the Jamiołkowski (14) isomorphism. In more general situations these techniques are not available, and one of us introduced in [3] an alternative approach to study positivity properties of maps of a C^*-algebra into $B(\mathcal{H})$. We now recall some of the definitions. For simplicity we continue to assume $\mathcal{H}$ is finite dimensional.

Let A be a C^*-algebra. Then there is a duality between bounded linear maps Φ of A into $B(\mathcal{H})$ and linear functionals $\tilde{\Phi}$ on $A \otimes B(\mathcal{H})$ given by

$$\tilde{\Phi}(a \otimes b) = \mathrm{Tr}\left(\Phi(a) b^t\right), \, a \in A, \, b \in B(\mathcal{H}), \tag{64}$$

where Tr is the usual trace on $B(\mathcal{H})$ and t the transpose. Furthermore, Φ is positive iff $\tilde{\Phi}$ is positive on the cone $A^+ \otimes B^+(\mathcal{H})$ of separable operators. We say a nonzero cone $\mathcal{K}$ in $\mathcal{P}(\mathcal{H})$ is a *mapping cone* if $\Phi \in \mathcal{K}$ implies $\Psi \circ \Phi \circ \Upsilon \in \mathcal{K}$ for all $\Psi, \Upsilon \in \mathcal{CP}(\mathcal{H})$. Well known examples are $\mathcal{P}(\mathcal{H})$, $\mathcal{CP}(\mathcal{H})$, the copositive maps and $\mathcal{SP}(\mathcal{H})$. We define

$$P(A, \mathcal{K}) := \{x \in A \otimes B(\mathcal{H}) \,|\, x = x^*, \mathbb{1} \otimes \Psi(x) \geqslant 0 \,\forall_{\Psi \in \mathcal{K}}\}, \tag{65}$$

where $\mathbb{1}$ denotes the identity map on $\mathcal{L}(\mathcal{H})$, $P(A, \mathcal{K})$ is a proper closed cone in $A \otimes B(\mathcal{H})$ containing the cone $A^+ \otimes B^+(\mathcal{H})$.

We say Φ is $\mathcal{K}$-*positive* if $\tilde{\Phi}$ is positive on $P(A, \mathcal{K})$, and denote by $\mathcal{P}_{\mathcal{K}}(\mathcal{H})$ the set of $\mathcal{K}$-positive maps of A into $B(\mathcal{H})$. Then Φ is completely positive iff Φ is $\mathcal{CP}(\mathcal{H})$-positive [3, Theorem 3.2] iff $\tilde{\Phi}$ is a positive linear functional on $A \otimes B(\mathcal{H})$.

If A is contained in a larger C^*-algebra B then $\mathcal{K}$-positive maps from A to $B(H)$ have $\mathcal{K}$-positive extensions to maps from B into $B(\mathcal{H})$, [3, Theorem 3.1]. In particular, this holds if $B = B(\mathcal{H})$. Therefore the results from the previous sections are applicable in much more general situations as soon as we can show $\mathcal{K} = \mathcal{P}_{\mathcal{K}}(\mathcal{H})$. The main results in the present section are concerned with this problem, and we shall show that it has an affirmative solution for the cones $\mathcal{P}_k(\mathcal{H})$, $\mathcal{SP}_k(\mathcal{H})$ and leave the discussion of $\mathcal{D}_{k,m}(\mathcal{H})$ and $\mathcal{S}_{k,m}(\mathcal{H})$ to the reader.

Lemma IV.1. *The cones $\mathcal{P}_k(\mathcal{H})$, $\mathcal{SP}_k(\mathcal{H})$, $\mathcal{D}_{k,m}(\mathcal{H})$ and $\mathcal{S}_{k,m}(\mathcal{H})$ are all mapping cones.*

Proof. If $\Phi \in \mathcal{P}_k(\mathcal{H})$ then $\mathbb{1}_k \otimes \Phi \geqslant 0$, where $\mathbb{1}_k$ is the identity map on a k-dimensional Hilbert space. Thus if $\Psi \in \mathcal{CP}(\mathcal{H})$,

$$\mathbb{1}_k \otimes (\Phi \circ \Psi) = (\mathbb{1}_k \otimes \Phi)(\mathbb{1}_k \otimes \Psi) \geqslant 0 \tag{66}$$

and

$$\mathbb{1}_k \otimes (\Psi \circ \Phi) = (\mathbb{1}_k \otimes \Psi)(\mathbb{1}_k \otimes \Phi) \geqslant 0. \tag{67}$$

Thus $\mathcal{P}_k(\mathcal{H})$ is a mapping cone. $\square$

If $\operatorname{rk} a \leqslant k$ then for all $b \in B(\mathcal{H})$, $\operatorname{rk} ab \leqslant k$ and $\operatorname{rk} ba \leqslant k$. Thus $\operatorname{Ad}_b \circ \operatorname{Ad}_a = \operatorname{Ad}_{ba} \in \mathcal{SP}_k(\mathcal{H})$, and $\operatorname{Ad}_a \circ \operatorname{Ad}_b \in \mathcal{SP}_k(\mathcal{H})$. It follows that $\mathcal{SP}_k(\mathcal{H})$ is a mapping cone. From the definitions of $\mathcal{D}_{k,m}(\mathcal{H})$ and $\mathcal{S}_{k,m}(\mathcal{H})$ it follows that they are also mapping cones.

Theorem IV.2. $\mathcal{SP}_k(\mathcal{H}) = \mathcal{P}_{\mathcal{SP}_k(\mathcal{H})}(\mathcal{H})$, and $\mathcal{P}_k(\mathcal{H}) = \mathcal{P}_{\mathcal{P}_k(\mathcal{H})}(\mathcal{H})$.

Proof. By Theorem III.12, $\Phi \in \mathcal{P}_k(\mathcal{H})$ iff $\Psi \circ \Phi \in \mathcal{CP}(\mathcal{H})$ for all $\Psi \in \mathcal{SP}_k(\mathcal{H})$. Hence by [47, Theorem 1], $\Phi \in \mathcal{P}_k(\mathcal{H})$ iff Φ belongs to the dual cone $\mathcal{P}_{\mathcal{SP}_k(\mathcal{H})}(\mathcal{H})^\circ$ of $\mathcal{P}_{\mathcal{SP}_k(\mathcal{H})}(\mathcal{H})$. By Proposition III.3, $\mathcal{P}_k(\mathcal{H}) = \mathcal{SP}_k(\mathcal{H})^\circ$. Thus $\mathcal{SP}_k(\mathcal{H}) = \mathcal{P}_k(\mathcal{H})^\circ = \mathcal{P}_{\mathcal{SP}_k(\mathcal{H})}(\mathcal{H})^{\circ\circ} = \mathcal{P}_{\mathcal{SP}_k(\mathcal{H})}(\mathcal{H})$, proving the first statement.

Similarly by Proposition III.4, $\Phi \in \mathcal{P}_k(\mathcal{H})^\circ$ iff $\Phi \in \mathcal{SP}_k(\mathcal{H})$. Thus by Theorem III.10, $\Phi \in \mathcal{P}_k(\mathcal{H})^\circ$ iff $\Psi \circ \Phi \in \mathcal{CP}(\mathcal{H})$ for all $\Psi \in \mathcal{P}_k(\mathcal{H})$, hence by Theorem 1 in [47] iff $\Phi \in \mathcal{P}_{\mathcal{P}_k(\mathcal{H})}(\mathcal{H})^\circ$. Thus $\mathcal{P}_k(\mathcal{H}) = \mathcal{P}_{\mathcal{P}_k(\mathcal{H})}(\mathcal{H})$. $\square$

Using the above theorem and its proof together with Theorem 1 in [47] we can add two more conditions to the equivalent conditions in Theorems III.10 and III.12,

Corollary IV.3. *The following conditions are equivalent for $\Phi \in \mathcal{E}(\mathcal{H})$,*

1) $\Phi \in \mathcal{P}_k(\mathcal{H})$, *i.e.* Φ *is k-positive,*

2) $\mathbb{1} \otimes \Psi(C_\Phi) \geqslant 0 \,\forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$,

3) $\tilde{\Phi} \circ (\mathbb{1} \otimes \Psi) \geqslant 0 \,\forall_{\Psi \in \mathcal{SP}_k(\mathcal{H})}$.

$\square$

Corollary IV.4. *The following conditions are equivalent for $\Phi \in \mathcal{E}(\mathcal{H})$,*

1) $\Phi \in \mathcal{SP}_k(\mathcal{H})$, *i.e.* Φ *is k-superpositive,*

2) $\mathbb{1} \otimes \Psi(C_\Phi) \geqslant 0 \,\forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$,

3) $\tilde{\Phi} \circ (\mathbb{1} \otimes \Psi) \geqslant 0 \,\forall_{\Psi \in \mathcal{P}_k(\mathcal{H})}$.

$\square$

Using Proposition II.7, it becomes evident that the condition 2) in Corollary IV.4 is the same as the k-positive maps criterion by Terhal and Horodecki [53]. For $k = 1$, we get the well known positive maps criterion by Horodeccy [15] (Horodeccy is the plural form of the name Horodecki). Corollary IV.3 provides us with an analogous characterization of the set of k-block positive operators: *An operator $a \in B(\mathcal{H} \otimes \mathcal{H})$ is k-block positive iff $(\mathbb{1} \otimes \Psi) a \geqslant 0$ for all k-superpositive maps Ψ.*

Furthermore, the main theorem in [49] is a version of Corollary IV.3, slightly modified to encompass 2-copositive maps. One can easily deduce from it that the set of one-undistillable states on $\mathcal{H} \otimes \mathcal{H}$ is precisely 2-$BP(\mathcal{H} \otimes \mathcal{H})$.

V.   CONCLUDING REMARKS

In this paper we studied the structure of the set of positive maps from the space $B(\mathcal{H})$ of linear operators on a finite-dimensional Hilbert space $\mathcal{H}$ into itself. This topic is of substantial interest in quantum physics, since positive maps are closely related to the separability problem due to the positive maps criterion by Horodeccy [15]. More generally, but less acute, positive maps are related to the separability problem because they correspond to hyperplanes that separate entangled states from the separable ones.

Here we developed general methods for proving results like the Horodeccy criterion, both in the situation where the Jamiołkowski isomorphism is at hand and within a more general setup, where other techniques need to be used, based on mapping cones (cf. Section IV). Our discussion concentrated on k-positive maps and on the dual cones of k-superpositive maps, consisting of completely positive maps that admit a Kraus representation by operators of rank $\leqslant k$ (such maps are also called *partially entanglement breaking channels*, [45]). We gave a number of characterization theorems (Theorems III.10, III.12, III.11, III.13 and Corollaries IV.3, IV.4) for both k-positive and k-superpositive maps, pertaining to their properties under taking compositions. Central to these results is the observation that a product of a k-superpositive map and a k-positive map is again a k-superpositive map (Theorem III.6). We have not seen that particular result anywhere in the literature. Also our characterization theorems seem to appear for the first time in this paper.

We introduced (similarly to [45], only using different notation) the cones of (k, m)-entangled, (k, m)-decomposable and (k, m)-positive maps ($\mathcal{S}_{k,m}(\mathcal{H})$, $\mathcal{D}_{k,m}(\mathcal{H})$ and $\mathcal{P}_{k,m}(\mathcal{H})$, respectively). The main results of this paper can be trivially generalized to these families of maps.

Most of our work relied on the simple and fine idea of *duality* between convex cones [54], which is nevertheless hard to grasp intuitively for spaces of dimension higher than 3 (it is not even completely trivial for three-dimensional

cones, see Figure 2). We hope that the figures we included in Section III could help the reader to develop basic intuitions about the geometric background to our work. On that occasion we touched upon the question of optimality of entanglement witnesses. By pointing out that the extreme points of the set of unital witnesses are optimal, we tried to spill the idea that future efforts could concentrate on witnesses which are not only optimal, but also extreme.

Within this paper several results by other authors [7, 11, 12, 15, 49, 53] appear as special cases of general theorems. Presented in the way we did it, they start to reveal a mathematical structure of a certain degree of generality. For a mathematican, it is natural to ask if there are many examples of this structure, or maybe it is very specific to the studied cones. In other words, the question is, how many are there interesting examples of mapping cones $\mathcal{K}$ in $\mathcal{L}(\mathcal{H})$ such that $\mathcal{P}_{\mathcal{K}}(\mathcal{H}) = \mathcal{K}$? We do not know the answer at the moment. From a physicist's perspective, the key question here is to what extend the families $\mathcal{S}_{k,m}(\mathcal{H})$, $\mathcal{D}_{k,m}(\mathcal{H})$ and $\mathcal{P}_{k,m}(\mathcal{H})$ can be useful in entanglement research and how our theorems can be applied in practice. The example of the paper [49] suggests that our discussion is not purely abstract and may relate to physically relevant questions like the distillability of entanglement.

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[60] A simpler proof of Proposition II.6 can be obtained by noting that the Choi matrix C_{Ad_a} is a positive rank one operator, and so are all the Choi matrices $C_{\mathrm{Ad}_{a_i}}$, hence the Ad_{a_i} are scalar multiples of Ad_a. We have kept the longer proof because of its connection with Lemma II.5

[61] The two propositions are not used in later parts of the paper, but they make for an apt comment to Figure 3.