Chapter 2

Detecting Quantum Entanglement: Positive Maps and Entanglement Witnesses

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Additional information is available at the end of the chapter

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1. Introduction

The interest on quantum entanglement has dramatically increased during the last 2 decades due to the emerging field of quantum information theory. It turns out that quantum entanglement may be used as basic resources in quantum information processing and communication. The prominent examples are quantum cryptography, quantum teleportation, quantum error correction codes, and quantum computation. Since the quantum entanglement is the basic resource for the new quantum information technologies, it is therefore clear that there is a considerable interest in efficient theoretical and experimental methods of entanglement detection.

One of the most important problems of quantum information theory [1–3] is the characterization of mixed states of composed quantum systems. In particular it is of primary importance to test whether a given quantum state exhibits quantum correlation, i.e. whether it is separable or entangled. For low-dimensional systems there exists simple necessary and sufficient condition for separability. The celebrated Peres-Horodecki criterion states that a state of a bipartite system living in $\mathbb{C}^2 \otimes \mathbb{C}^2$ or $\mathbb{C}^2 \otimes \mathbb{C}^3$ is separable iff its partial transpose is positive. Unfortunately, for higher-dimensional systems there is no single *universal* separability condition.

It turns out that the above problem may be reformulated in terms of positive linear maps in operator algebras [4]: a state ρ in $\mathcal{H}_1 \otimes \mathcal{H}_2$ is separable iff $(\mathrm{id} \otimes \varphi)\rho$ is positive for any positive map φ which sends positive operators on $\mathcal{H}_2$ into positive operators on $\mathcal{H}_1$. Therefore, a classification of positive linear maps between operator algebras $\mathcal{B}(\mathcal{H}_1)$ and $\mathcal{B}(\mathcal{H}_2)$ is of primary importance. Unfortunately, in spite of the considerable effort, the structure of positive maps is still poorly understood (see "classical" papers on positive maps [5]–[17] and some recent papers [18]–[63]).

In this paper we provide characterization of important classes of positive maps in finite dimensional matrix algebras. Equivalently, due to the Choi-Jamiołkowski isomorphism, we characterized the corresponding classes of entanglement witnesses. Concerning the application in quantum entanglement theory the key role is played by indecomposable witnesses which can detect PPT entangled states, that is, a PPT state ρ_{AB} is entangled iff there exists an indecomposable entanglement witness W such that $\mathrm{Tr}(W\rho) < 0$. We illustrate the general presentation with several examples of indecomposable positive maps/entanglement witnesses: the Choi-like maps in $M_3(\mathbb{C})$, its generalizations in $M_d(\mathbb{C})$, and the Robertson map in $M_4(\mathbb{C})$ together with its generalizations in $M_{2k}(\mathbb{C})$. These examples enables one to discuss several properties like optimality and/or exposedness which are crucial in entanglement theory.

2. Positive maps and entanglement witnesses

In this paper we restrict our analysis to linear maps

$$\Lambda : M_d(\mathbb{C}) \ \rightarrow \ M_d(\mathbb{C}) \ , \tag{1}$$

where $M_d(\mathbb{C})$ denotes a set of $d \times d$ complex matrices. Let $M_d(\mathbb{C})^+$ be a convex set of semi-positive elements in $M_d(\mathbb{C})$.

Definition 1. *One calls Λ a positive map if $\Lambda a \in M_d(\mathbb{C})^+$ for any $a \in M_d(\mathbb{C})^+$. Similarly, Λ is k-positive if*

$$\Lambda_{(k)} := \mathrm{id}_k \otimes \Lambda \ : M_k(\mathbb{C}) \otimes M_d(\mathbb{C}) \longrightarrow \ M_k(\mathbb{C}) \otimes M_d(\mathbb{C}) \ , \tag{2}$$

is positive. Finally, Λ is completely positive (CP) if it is k-positive for all k.

Let $\mathcal{P}_k$ denotes a convex set of k-positive maps in $M_d(\mathbb{C})$. One has $\mathcal{P}_k \subset \mathcal{P}_l$ for $k > l$. Actually, due to the Choi theorem any d-positive map in $M_d(\mathbb{C})$ is CP, and hence $\mathcal{P}_{\mathrm{CP}} = \mathcal{P}_d$. Therefore, one has the following chain of proper inclusions

$$\mathcal{P}_{\mathrm{CP}} \subset \mathcal{P}_{d-1} \subset \ldots \subset \mathcal{P}_1 \ , \tag{3}$$

where $\mathcal{P}_1$ denotes a set of all positive maps in $M_d(\mathbb{C})$. Let $\{e_1, \ldots, e_d\}$ denotes an orthonormal basis in $\mathbb{C}^d$, and let "T" denotes a transposition map with respect to this basis, i.e. for any $a = \sum_{ij} a_{ij} e_{ij}$ one has $T(a) = \sum_{ij} a_{ij} e_{ji}$, where $e_{ij} := |e_i\rangle\langle e_j|$.

Definition 2. *One calls a linear map Λ k-copositive if the map $\Lambda \circ \mathrm{T}$ is k-positive.*

Let $\mathcal{P}^k$ denotes a convex set of k-copositive maps. One has

$$\mathcal{P}^{\mathrm{CP}} \subset \mathcal{P}^{d-1} \subset \ldots \subset \mathcal{P}^1 \ , \tag{4}$$

where $\mathcal{P}^1$ denotes a set of all copositive maps in $M_d(\mathbb{C})$, and $\mathcal{P}^{\mathrm{CP}}$ stands for a set of completely copositive maps (CcP). Let $\mathcal{P}_l^k$ denotes a set of maps which are l-positive and k-copositive. One has the following relations

$$\mathcal{P}_{\mathrm{CP}}^{\mathrm{CP}} \subset \mathcal{P}_{d-1}^{d-1} \subset \ldots \subset \mathcal{P}_1^1 \ . \tag{5}$$

Definition 3. *A positive map* $\Lambda \in \mathcal{P}_1$ *is called* decomposable *if*

$$\Lambda = \Lambda_1 + \Lambda_2 \ , \tag{6}$$

where $\Lambda_1 \in \mathcal{P}_{\mathrm{CP}}$ *and* $\Lambda_2 \in \mathcal{P}^{\mathrm{CP}}$*. A map which is not decomposable is called* indecomposable*. A positive map* $\Lambda \in \mathcal{P}_1$ *is called* atomic *if it cannot be written as in (6), where* $\Lambda_1 \in \mathcal{P}_2$ *and* $\Lambda_2 \in \mathcal{P}^2$*.*

It is clear that each atomic map is indecomposable but the converse is not true. Since $\mathcal{P}_1$ is a convex set it is fully characterized by its extreme elements. Clearly a positive map Λ is *extremal* if for any $\Psi \in \mathcal{P}_1$, a map $\Lambda - \Psi$ is not positive. Finally, a positive map Λ is *optimal* if for any $\Psi \in \mathcal{P}_{\mathrm{CP}}$, a map $\Lambda - \Psi$ is not positive. It is evident that each extremal map is optimal but the converse is not true.

The vectors spaces of linear maps in $M_d(\mathbb{C})$ and linear operators in $M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$ have the same dimensions d^2, and hence they are isomorphic. Fixing an orthonormal basis $\{e_1, \ldots, e_d\}$ in $\mathbb{C}^d$ one may establish the following isomorphism known in the quantum information community as the *Choi-Jamiołkowski isomorphism*.

Theorem 1. *A space of linear maps in* $M_d(\mathbb{C})$ *is isomorphic to the space of linear operators in* $M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$*. The corresponding isomorphism is provided by the following formula: for a linear map* Λ *one defines a linear operator* $W_\Lambda \in M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$*:*

$$W_\Lambda = (\mathrm{id} \otimes \Lambda) P_d^+ \ , \tag{7}$$

where P_d^+ *denotes a canonical maximally entangled state in* $\mathbb{C}^d \otimes \mathbb{C}^d$

$$P_d^+ = \frac{1}{d} \sum_{i,j=1}^{d} e_{ij} \otimes e_{ij} \ . \tag{8}$$

The inverse formula reads

$$\Lambda_W(a) = d\, \mathrm{Tr}_2(W \cdot [\mathbb{I}_d \otimes T(a)]) \ . \tag{9}$$

Actually, it is inner product isomorphism, that is,

$$\langle\langle \Lambda_A | \Lambda_B \rangle\rangle = \langle A | B \rangle \ , \tag{10}$$

where $\langle A|B \rangle = \mathrm{Tr}(A^\dagger B)$ *, and*

$$\langle\langle \Lambda_A | \Lambda_B \rangle\rangle = \sum_{\alpha=1}^{d^2} \langle \Lambda_A(f_\alpha) | \Lambda_B(f_\alpha) \rangle \ , \tag{11}$$

with f_α *being an orthonormal basis in* $M_d(\mathbb{C})$*, i.e.* $\langle f_\alpha | f_\beta \rangle = \delta_{\alpha\beta}$*.*

Now, if Λ is a linear map preserving hermicity, that is, $\Lambda(X^\dagger) = [\Lambda(X)]^\dagger$, then W_Λ is hermitian [8]. If Λ is a positive map, then W_Λ satisfies [9]

$$\langle \psi \otimes \phi | W | \psi \otimes \phi \rangle \geq 0 \, , \tag{12}$$

for all $\psi, \phi \in \mathbb{C}^d$. Moreover, if Λ is CP, then $W_\Lambda \geq 0$ [10], that is,

$$\langle \Psi | W | \Psi \rangle \geq 0 \, , \tag{13}$$

for all $\Psi \in \mathbb{C}^d \otimes \mathbb{C}^d$. It is clear that (13) implies (12) but not vice versa. An operator satisfying (12) is called block-positive.

Definition 4. *A block-positive but not positive operator W is called an entanglement witness.*

It is clear that due to the Choi-Jamiołkowski isomorphism one can translate all properties of linear maps into the corresponding properties of linear operators $W \in M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$. In particular one has

Definition 5. *An entanglement witness W is decomposable iff*

$$W = W_1 + W_2^\Gamma \, , \tag{14}$$

where $W_1, W_2 \geq 0$ and $A^\Gamma = (\mathrm{id} \otimes T)A$ denotes partial transposition.

Let $\mathcal{D}$ be a subset of density operators of a composite quantum system living in $\mathbb{C}^n \otimes \mathbb{C}^n$ detected by a given EW W, that is, $\mathcal{D} = \{\rho \mid \mathrm{Tr}(W\rho) < 0\}$. Given two EWs W_1 and W_2 one says that W_2 is finer than W_1 if $\mathcal{D}_1 \subset \mathcal{D}_2$, that is, all states detected by W_1 are also detected by W_2. A witness W is optimal if there is no other EW which is finer than W. It means that W detects quantum entanglement in the 'optimal way'. It is clear that the knowledge of optimal EWS is crucial to classify quantum states of composite systems. One proves the following

Proposition 1. *W is an optimal EW if and only if $W - Q$ is no longer EW for arbitrary positive operator Q.*

Authors of Ref. [32] formulated the following criterion for the optimality of W.

Proposition 2. *If the set of product vectors $x \otimes y \in \mathbb{C}^n \otimes \mathbb{C}^n$ satisfying*

$$\langle x \otimes y | W | x \otimes y \rangle = 0 \, , \tag{15}$$

span the total Hilbert space $\mathbb{C}^n \otimes \mathbb{C}^n$, then W is optimal.

The further classification of entanglement witnesses would be provided in the next section.

3. States of composite quantum systems

Let $\Psi \in \mathbb{C}^d \otimes \mathbb{C}^d$ such that $\langle\Psi|\Psi\rangle = 1$, and consider the corresponding Schmidt decomposition

$$\Psi = \sum_{k=1}^{r} \mu_k \, e_k \otimes f_k \ , \tag{16}$$

where $\mu_k > 0$ and $\sum_{k=1}^{r} \mu_k^2 = 1$. In the above formula $\{e_i\}$ and $\{f_j\}$ are two mutually orthogonal normalized vectors in $\mathbb{C}^d$. One calls the number r the Schmidt rank of Ψ – $SR(\Psi)$. It is clear that $1 \le r \le d$. Consider now a density operator $\rho \in M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$.

Definition 6. *A Schmidt number [31] of* ρ *–* $SN(\rho)$ *– is defined by*

$$SN(\rho) = \min_{p_k,\psi_k} \left\{ \max_k \, SR(\Psi_k) \right\} \ , \tag{17}$$

where the minimum is taken over all possible pure states decompositions

$$\rho = \sum_k p_k \, |\Psi_k\rangle\langle\Psi_k| \ , \tag{18}$$

with $p_k \ge 0$*,* $\sum_k p_k = 1$ *and* Ψ_k *are normalized vectors in* $\mathbb{C}^d \otimes \mathbb{C}^d$*.*

Let us introduce the following family of positive cones:

$$\mathrm{V}_r = \{ \rho \in (M_d \otimes M_d)^+ \mid \mathrm{SN}(\rho) \le r \} \ . \tag{19}$$

One has the following chain of inclusions

$$\mathrm{V}_1 \subset \ldots \subset \mathrm{V}_d \equiv (M_d \otimes M_d)^+ \ . \tag{20}$$

Clearly, V_1 is a cone of separable (unnormalized) states and $V_d \setminus V_1$ stands for a set of entangled states. Note, that a partial transposition $(\mathrm{id} \otimes \mathrm{T})$ gives rise to another family of cones:

$$\mathrm{V}^l = (\mathrm{id} \otimes \mathrm{T})\mathrm{V}_l \ , \tag{21}$$

such that $\mathrm{V}^1 \subset \ldots \subset \mathrm{V}^d$. One has $\mathrm{V}_1 = \mathrm{V}^1$, together with the following hierarchy of inclusions:

$$\mathrm{V}_1 = \mathrm{V}_1 \cap \mathrm{V}^1 \subset \mathrm{V}_2 \cap \mathrm{V}^2 \subset \ldots \subset \mathrm{V}_d \cap \mathrm{V}^d \ . \tag{22}$$

Note, that $\mathrm{V}_d \cap \mathrm{V}^d$ is a convex set of PPT (unnormalized) states. Finally, $\mathrm{V}_r \cap \mathrm{V}^s$ is a convex subset of PPT states ρ such that $\mathrm{SN}(\rho) \le r$ and $\mathrm{SN}(\rho^\Gamma) \le s$.

Proposition 3. *Let $\Lambda : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ be a linear map. $\Lambda \in \mathcal{P}_k$ if and only if*

$$(\mathrm{id} \otimes \Lambda) V_k \subset V_d \ . \tag{23}$$

$\Lambda \in \mathcal{P}^k$ if and only if

$$(\mathrm{id} \otimes \Lambda) V^k \subset V_d \ . \tag{24}$$

Finally, $\Lambda \in \mathcal{P}_l^k$ if and only if

$$(\mathrm{id} \otimes \Lambda) V^k \cap V_l \subset V_d \ . \tag{25}$$

Let us denote by W a space of entanglement witnesses, i.e. a space of non-positive Hermitian operators $W \in M_d \otimes M_d$ such that $\mathrm{Tr}(W\rho) \geq 0$ for all $\rho \in \mathrm{V}_1$. Define a family of subsets $\mathrm{W}_r \subset M_d \otimes M_d$:

$$\mathrm{W}_r = \{ \, W \in M_d \otimes M_d \mid \mathrm{Tr}(W\rho) \geq 0 \ , \ \rho \in \mathrm{V}_r \, \} \ . \tag{26}$$

One has

$$(M_d \otimes M_d)^+ \equiv \mathrm{W}_d \subset \ldots \subset \mathrm{W}_1 \ . \tag{27}$$

Clearly, $\mathrm{W} = \mathrm{W}_1 \smallsetminus \mathrm{W}_d$. Moreover, for any $k > l$, entanglement witnesses from $\mathrm{W}_l \smallsetminus \mathrm{W}_k$ can detect entangled states from $\mathrm{V}_k \smallsetminus V_l$, i.e. states ρ with Schmidt number $l < \mathrm{SN}(\rho) \leq k$. In particular $W \in \mathrm{W}_k \smallsetminus \mathrm{W}_{k+1}$ can detect state ρ with $\mathrm{SN}(\rho) = k$.

Consider now the following class of witnesses

$$\mathrm{W}_r^s := \mathrm{W}_r + (\mathrm{id} \otimes \mathrm{T})\mathrm{W}_s \ , \tag{28}$$

that is, $W \in \mathrm{W}_r^s$ iff

$$W = P + Q^\Gamma \ , \tag{29}$$

with $P \in \mathrm{W}_r$ and $Q \in \mathrm{W}_s$. Note, that $\mathrm{Tr}(W\rho) \geq 0$ for all $\rho \in \mathrm{V}_r \cap \mathrm{V}^s$. Hence such W can detect PPT states ρ such that $\mathrm{SN}(\rho) \geq r$ or $\mathrm{SN}(\rho^\Gamma) \geq s$.

Proposition 4. *Elements from W_d^d are decomposable entanglement witnesses.*

It is clear that decomposable entanglement witnesses cannot detect PPT states. One has the following chain of inclusions:

$$\mathrm{W}_d^d \subset \ldots \subset \mathrm{W}_2^2 \subset \mathrm{W}_1^1 \equiv \mathrm{W} \ . \tag{30}$$

The 'weakest' entanglement can be detected by elements from $\mathrm{W}_1^1 \smallsetminus \mathrm{W}_2^2$. We shall call them *atomic entanglement witnesses*.

Let $\mathcal{P}_1^\circ$ denote a dual cone [23, 64] to the convex cone $\mathcal{P}_1$ of positive maps

$$\mathcal{P}^\circ = \mathrm{conv}\{ \, P_x \otimes P_y \, ; \, \langle y|\Phi(P_x)|y\rangle \geq 0 \, , \, \Phi \in \mathcal{P}_1 \, \} \, , \tag{31}$$

where $P_x = |x\rangle\langle x|$ and $P_y = |y\rangle\langle y|$. It is clear that $\mathcal{P}_1^{\circ\circ} = \mathcal{P}_1$, that is, one may consider $\mathcal{P}_1$ as a dual cone to the convex cone of separable operators in $\mathcal{H} \otimes \mathcal{H}$. Recall that a face of $\mathcal{P}_1$ is a convex subset $F \subset \mathcal{P}_1$ such that if the convex combination $\Phi = \lambda\Phi_1 + (1-\lambda)\Phi_2$ of $\Phi_1, \Phi_2 \in \mathcal{P}_1$ belongs to F, then both $\Phi_1, \Phi_2 \in F$. If a ray $\{\lambda\Phi \, : \, \lambda > 0\}$ is a face of $\mathcal{P}_1$ then it is called an extreme ray, and we say that Φ generates an extreme ray. For simplicity we call such Φ an extremal positive map. A face F is exposed if there exists a supporting hyperplane H for a convex cone $\mathcal{P}$ such that $F = H \cap \mathcal{P}_1$.

A positive map $\Phi \in \mathcal{P}_1$ is exposed if it generates 1-dimensional exposed face. Let us denote by $\mathrm{Ext}(\mathcal{P}_1)$ the set of extremal points and $\mathrm{Exp}(\mathcal{P}_1)$ the set of exposed points of $\mathcal{P}_1$. Due to Straszewicz theorem [64] $\mathrm{Exp}(\mathcal{P}_1)$ is a dense subset of $\mathrm{Ext}(\mathcal{P}_1)$. Thus every extreme map is the limit of some sequence of exposed maps meaning that each entangled state may be detected by some exposed positive map. Hence, a knowledge of exposed maps is crucial for the full characterization of separable/entangled states of bi-partite quantum systems.

4. Choi-like maps in $M_3(\mathbb{C})$

It is well known that all positive maps $\Lambda : M_2(\mathbb{C}) \to M_2(\mathbb{C})$, $\Lambda : M_2(\mathbb{C}) \to M_3(\mathbb{C})$ and $\Lambda : M_3(\mathbb{C}) \to M_2(\mathbb{C})$ are decomposable [5, 12]. The first example of an indecomposable positive linear map in $M_3(\mathbb{C})$ was found by Choi [10]. The (normalized) Choi map reads as follows

$$\begin{aligned} \Phi_C(e_{ii}) &= \sum_{i,j=1}^{3} A_{ij}^{C} e_{jj} \, , \\ \Phi_C(e_{ij}) &= -\frac{1}{2} e_{ij} \, , \quad i \neq j \, , \end{aligned} \tag{32}$$

where $||A_{ij}^C||$ is the following doubly stochastic matrix:

$$A_{ij}^C = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \, . \tag{33}$$

Let us consider a class of positive maps in $M_4(\mathbb{C})$ defined as follows [20]

$$\Phi[a,b,c] = N_{abc}(D[a,b,c] - \mathrm{id}) \, , \tag{34}$$

where $D[a,b,c]$ is a completely positive linear map defined by

$$D[a,b,c](X) = \begin{pmatrix} y_1 & 0 & 0 \\ 0 & y_2 & 0 \\ 0 & 0 & y_3 \end{pmatrix} , \tag{35}$$

and

$$\begin{aligned} y_1 &= (a+1)x_{11} + bx_{22} + cx_{33} , \\ y_2 &= cx_{11} + (a+1)x_{22} + bx_{33} , \\ y_3 &= bx_{11} + cx_{22} + (a+1)x_{33} , \end{aligned}$$

with x_{ij} being the matrix elements of $X \in M_3(\mathbb{C})$. The normalization factor $N_{abc} = (a+b+c)^{-1}$ guarantees that $\Phi[a,b,c]$ is unital, i.e. $\Phi[a,b,c](\mathbb{I}_3) = \mathbb{I}_3$. Note, that $\Phi[a,b,c]$ gives rise to the following doubly stochastic circulant matrix

$$D = N_{abc} \begin{pmatrix} a & b & c \\ c & a & b \\ b & c & a \end{pmatrix} . \tag{36}$$

This family contains well known examples of positive maps: note that $\Phi[0,1,1](X) = \frac{1}{2}(\mathrm{Tr}X\,\mathbb{I}_3 - X)$ which reproduces the reduction map. Moreover, $\Phi[1,1,0]$ and $\Phi[1,0,1]$ reproduce Choi map and its dual, respectively. One proves the following result [20]

Theorem 2. *A map $\Phi[a,b,c]$ is positive but not completely positive if and only if*

1. $0 \le a < 2$,
2. $a+b+c \ge 2$,
3. *if* $a \le 1$, *then* $bc \ge (1-a)^2$.

Moreover, being positive it is indecomposable if and only if $4bc < (2-a)^2$.

Actually, $\Phi[a,b,c]$ is indecomposable if and only if it is atomic, i.e. it cannot be decomposed into the sum of 2-positive and 2-copositive maps. The corresponding entanglement witness reads as follows

$$W[a,b,c] = N_{abc} \sum_{i,j=1}^{3} e_{ij} \otimes W_{ij} , \tag{37}$$

with

$$\begin{aligned} W_{11} &= ae_{11} + be_{22} + ce_{33} , \\ W_{22} &= ce_{11} + ae_{22} + be_{33} , \\ W_{33} &= be_{11} + ce_{22} + ae_{33} , \\ W_{ij} &= -e_{ij} , \quad i \neq j . \end{aligned}$$

In a recent paper [54] we analyzed a special case corresponding to $a+b+c=2$. It turns out [54] that $\Phi[a,b,c]$ is parameterized by the ellipse on the bc-plane. Moreover, one proves the following

Theorem 3 ([56, 57]). *A map $\Phi[a,b,c]$ with $a+b+c=2$ is optimal iff $a \leq 1$. It is indecomposable iff $a > 0$.*

Interestingly

Theorem 4 ([58]). *A map $\Phi[a,b,c]$ with $a+b+c=2$ is exposed iff $0 < a < 1$.*

Interestingly, indecomposability of these maps may be proved by using the following family of PPT states in $\mathbb{C}^3 \otimes \mathbb{C}^3$:

$$\rho_\epsilon = N_\epsilon \left(\sum_{i,j=1}^{3} e_{ij} \otimes e_{ij} + \epsilon \sum_{i=1}^{3} e_{ii} \otimes e_{i+1,i+1} + \epsilon^{-1} \sum_{i=1}^{3} e_{ii} \otimes e_{i+2,i+2} \right) , \tag{38}$$

with $\epsilon > 0$ and $N_\epsilon = [3(1+\epsilon+\epsilon^{-1})]^{-1}$. It is well known that ρ_ϵ is entangled iff $\epsilon \neq 1$.

5. Indecomposable maps in $M_d(\mathbb{C})$ — generalized Choi maps

In this section we provide several examples of positive maps in $M_d(\mathbb{C})$ which generalize Choi map in $M_3(\mathbb{C})$.

Example 1. The Choi map in $M_3(\mathbb{C})$ may be generalized to a positive map in $M_d(\mathbb{C})$ as follows [24]: let S be a unitary shift defined by:

$$S\, e_i = e_{i+1} \ , \qquad i = 1, \ldots, d \ ,$$

where the indices are understood mod d. One defines

$$\tau_{d,k}(X) = (d-k)\,\epsilon(X) + \sum_{i=1}^{k} \epsilon(S^i\, X\, S^{*i}) - X \ , \qquad k = 0,1,2,\ldots,d-1 \ , \tag{39}$$

where $\epsilon(X)$ denotes the following projector

$$\epsilon(X) = \sum_{k=1}^{d} e_{kk} X e_{kk} \ .$$

The map $\tau_{d,0}$ defined is completely positive and the map $\tau_{d,d-1}$ reproduces the reduction map in $M_d(\mathbb{C})$ (and hence it is completely copositive). Note that $\tau_{d,k}(\mathbb{I}_d) = (d-1)\mathbb{I}_d$, and $\mathrm{Tr}\, \tau_{d,k}(X) = (d-1)\mathrm{Tr}\, X$, hence the normalized maps

$$\Phi_{d,k}(X) = \frac{1}{d-1}\, \tau_{d,k}(X) \ , \tag{40}$$

are doubly stochastic. In particular $\Phi[1,0,1] = \Phi_{3,1}$.

Example 2. A class of maps $\varphi_{\mathbf{p}}$ parameterized by $d+1$ parameters $\mathbf{p} = (p_0, p_1, \ldots, p_d)$:

$$\begin{aligned} \Phi[\mathbf{p}](e_{11}) &= p_0 e_{11} + p_d e_{dd} \;, \\ \Phi[\mathbf{p}](e_{22}) &= p_0 e_{22} + p_1 e_{11} \;, \\ &\vdots \\ \Phi[\mathbf{p}](e_{dd}) &= p_0 e_{dd} + p_{d-1} e_{d-1,d-1} \;, \\ \Phi[\mathbf{p}](e_{ij}) &= -e_{ij} \;, \quad i \neq j \;. \end{aligned} \tag{41}$$

One proves

Theorem 5 ([19, 25]). *If* $\mathbf{p} = (p_0, p_1, \ldots, p_d)$ *satisfy*

$$\begin{aligned} &a) \quad p_1, \ldots, p_d > 0 \;, \\ &b) \quad d-1 > p_0 \geq d-2 \;, \\ &c) \quad p_1 \cdot \ldots \cdot p_d \geq (d-1-p_0)^d \;, \end{aligned}$$

then $\Phi[\mathbf{p}]$ *is a positive indecomposable map.*

Actually, $\Phi[\mathbf{p}]$ is atomic, i.e. it cannot be decomposed into the sum of a 2-positive and 2-copositive maps. In particular the corresponding EW for $d = 3$ reads as follows

$$W[\mathbf{p}] = N[\mathbf{p}] \sum_{i,j=1}^{3} e_{ij} \otimes W_{ij} \;, \tag{42}$$

with

$$\begin{aligned} W_{11} &= p_0 e_{11} + p_3 e_{33} \;, \\ W_{22} &= p_0 e_{22} + p_1 e_{11} \;, \\ W_{33} &= p_0 e_{33} + p_2 e_{22} \;, \\ W_{ij} &= -e_{ij} \;, \quad i \neq j \;, \end{aligned}$$

and the normalization factor reads $N[\mathbf{p}] = (3p_0 + p_1 + p_2 + p_3)^{-1}$. In particular if $p_1 = p_2 = p_3 = c$, then $W[\mathbf{p}] = W[p_0, 0, c]$.

6. Entanglement witnesses based on spectral conditions

Any entanglement witness W can be represented as a difference $W = W_+ - W_-$, where both W_+ and W_- are semi-positive operators in $\mathbb{C}^d \otimes \mathbb{C}^d$. However, there is no general method to recognize that W defined by $W_+ - W_-$ is indeed an EW. One particular method based on spectral properties of W was presented in [42]. Let ψ_α ($\alpha = 1, \ldots, D = d^2$) be an orthonormal basis in $\mathbb{C}^d \otimes \mathbb{C}^d$ and denote by P_α the corresponding projector $P_\alpha = |\psi_\alpha\rangle\langle\psi_\alpha|$. It leads therefore to the following spectral resolution of identity

$$\mathbb{I}_d \otimes \mathbb{I}_d = \sum_{\alpha=1}^{D} P_\alpha \ . \tag{43}$$

Having defined eigenvectors of W one needs the corresponding eigenvalues: let $\lambda_\alpha^- \leq 0$, for $\alpha = 1, \ldots, L < D$, and $\lambda_\alpha^+ > 0$ for $\alpha = L+1, \ldots, D$, that is,

$$W_- = -\sum_{\alpha=1}^{L} \lambda_\alpha^- P_\alpha \ , \quad W_+ = \sum_{\alpha=L+1}^{D} \lambda_\alpha^+ P_\alpha \ .$$

Let us analyze the condition for the spectrum $\{\lambda_\alpha^-, \lambda_\alpha^+\}$ which guarantees that W is block positive. Consider a normalized vector $\psi \in \mathbb{C}^d \otimes \mathbb{C}^d$ and let $s_1(\psi) \geq \ldots \geq s_d(\psi)$ denote its Schmidt coefficients. For any $1 \leq k \leq d$ one defines k-norm of ψ by the following formula

$$||\psi||_k^2 = \sum_{j=1}^{k} s_j^2(\psi) \ . \tag{44}$$

It is clear that $||\psi||_1 \leq ||\psi||_2 \leq \ldots \leq ||\psi||_d$. Note that $||\psi||_1$ gives the maximal Schmidt coefficient of ψ, whereas due to the normalization, $||\psi||_d^2 = \langle\psi|\psi\rangle = 1$. In particular, if ψ is maximally entangled then

$$||\psi||_k^2 = \frac{k}{d} \ . \tag{45}$$

Equivalently one may define k-norm of ψ by

$$||\psi||_k^2 = \max_{\phi} |\langle\psi|\phi\rangle|^2 \ , \tag{46}$$

where the maximum runs over all normalized vectors ϕ such that $\mathrm{SR}(\psi) \leq k$ (such ϕ is usually called k-separable). Recall that a Schmidt rank of ψ – $\mathrm{SR}(\psi)$ – is the number of non-vanishing Schmidt coefficients of ψ. One calls entanglement witness W a k-EW if $\langle\psi|W|\psi\rangle \geq 0$ for all ψ such that $\mathrm{SR}(\psi) \leq k$. One has the the following

Theorem 6 ([42]). *Let $\sum_{\alpha=1}^{L} ||\psi_\alpha||_k^2 < 1$. If the following spectral conditions are satisfied*

$$\lambda_\alpha^+ \geq \mu_k \ , \quad \alpha = L+1, \ldots, D \ , \tag{47}$$

where

$$\mu_\ell := \frac{\sum_{\alpha=1}^{L} |\lambda_\alpha^-| ||\psi_\alpha||_\ell^2}{1 - \sum_{\alpha=1}^{L} ||\psi_\alpha||_\ell^2} \ , \tag{48}$$

then W is an k-EW. If moreover $\sum_{\alpha=1}^{L} ||\psi_\alpha||_{k+1}^2 < 1$ *and*

$$\mu_{k+1} > \lambda_\alpha^+ \ , \quad \alpha = L+1, \ldots, D \ , \tag{49}$$

then W being k-EW is not $(k+1)$*-EW.*

Interestingly, one has the following

Theorem 7. $W = W_+ - W_-$ *is a decomposable EW.*

The proof is easy [43]: note that $W = A + B$, where

$$A = \sum_{\alpha=L+1}^{D} (\lambda_\alpha^+ - \mu_1) P_\alpha \ , \tag{50}$$

and

$$B = \mu_1 \mathbb{I}_d \otimes \mathbb{I}_d - \sum_{\alpha=1}^{L} (|\lambda_\alpha^-| + \mu_1) P_\alpha \ . \tag{51}$$

Now, since $\lambda_\alpha^+ \geq \mu_1$, for $\alpha = L+1, \ldots, D$, it is clear that $A \geq 0$. The partial transposition of B reads as follows

$$B^\Gamma = \mu_1 \mathbb{I}_d \otimes \mathbb{I}_d - \sum_{\alpha=1}^{L} (|\lambda_\alpha^-| + \mu_1) P_\alpha^\Gamma \ . \tag{52}$$

Let us recall that the spectrum of the partial transposition of rank-1 projector $|\psi\rangle\langle\psi|$ is well know: the nonvanishing eigenvalues of $|\psi\rangle\langle\psi|^\Gamma$ are given by $s_\alpha^2(\psi)$ and $\pm s_\alpha(\psi) s_\beta(\psi)$, where $s_1(\psi) \geq \ldots \geq s_d(\psi)$ are Schmidt coefficients of ψ. Therefore, the smallest eigenvalue of B^Γ (call it $b_{\min}$) satisfies

$$b_{\min} \geq \mu_1 - \sum_{\alpha=1}^{L} (|\lambda_\alpha^-| + \mu_1) ||\psi_\alpha||_1^2 \ , \tag{53}$$

and using the definition of μ_1 (cf. Eq. (48)) one gets $b_{\min} \geq 0$ which implies $B^\Gamma \geq 0$. Hence, the entanglement witness W is decomposable.

Remark 1. Interestingly, saturating the bound (47), i.e. taking

$$\lambda_\alpha^+ = \mu_1 \ , \quad \alpha = L+1, \ldots, D \ , \tag{54}$$

one has $A = 0$ and hence $W = Q^\Gamma$ with $Q = B^\Gamma \geq 0$ which shows that the corresponding positive map $\Lambda : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ defined by

$$\Lambda(X) = \mathrm{Tr}_1(W \cdot X^T \otimes \mathbb{I}_d) \ , \tag{55}$$

is completely co-positive. Note that

$$\Lambda(X) = \mu_1 \mathbb{I}_d \mathrm{Tr}\, X - \sum_{\alpha=1}^{L} (\mu_1 + |\lambda_\alpha|) F_\alpha X F_\alpha^\dagger \ , \tag{56}$$

where F_α is a linear operator $F_\alpha : \mathbb{C}^d \to \mathbb{C}^d$ defined by

$$\psi_\alpha = \sum_{i=1}^{d} e_i \otimes F_\alpha e_i \ , \tag{57}$$

and $\{e_1, \ldots, e_d\}$ denotes an orthonormal basis in $\mathbb{C}^d$. In particular, if $L = 1$, i.e. there is only one negative eigenvalue, then formula (56) (up to trivial rescaling) gives

$$\Lambda(X) = \kappa\, \mathbb{I}_d \mathrm{Tr}\, X - F_1 X F_1^\dagger \ , \tag{58}$$

with

$$\kappa = \frac{\mu_1}{\mu_1 + |\lambda_1|} = ||\psi_1||_1^2 \ . \tag{59}$$

It reproduces a positive map (or equivalently an EW $W = \kappa\, \mathbb{I}_d \otimes \mathbb{I}_d - P_1$) which is known to be completely co-positive [3, 39, 43]. If ψ_1 is maximally entangled, that is, $F_1 = U/\sqrt{d}$ for some unitary $U \in U(d)$, then one finds for $\kappa = 1/d$ and the map (58) is unitary equivalent to the reduction map $\Lambda(X) = UR(X)U^\dagger$, where $R_d(X) = \mathbb{I}_d \mathrm{Tr} X - X$.

Example 3. Consider an EW corresponding to the flip operator in $d = 2$:

$$W = e_{11} \otimes e_{11} + e_{22} \otimes e_{22} + e_{12} \otimes e_{21} + e_{21} \otimes e_{12} \ . \tag{60}$$

Its spectral decomposition has the following form

$$\psi_1 = \frac{1}{\sqrt{2}}(|12\rangle - |21\rangle) \ , \ \ \psi_2 = \frac{1}{\sqrt{2}}(|12\rangle + |21\rangle) \ , \ \ \psi_3 = |11\rangle \ , \ \ \psi_4 \ = \ |22\rangle \ .$$

together with the corresponding eigenvalues

$$-\lambda_1^- = \lambda_2^+ = \lambda_3^+ = \lambda_4^+ = 1 \ ,$$

One finds $\mu_1 = 1$ and hence condition (47) is trivially satisfied $\lambda_\alpha^+ \geq \mu_1$ for $\alpha = 2, 3, 4$. We stress that our construction does not recover flip operator in $d > 2$. It has $d(d-1)/2$ negative eigenvalues. Our construction leads to at most $d - 1$ negative eigenvalues.

7. Bell-diagonal entanglement witnesses

Let us define a generalized Bell states [65] in $\mathbb{C}^d \otimes \mathbb{C}^d$

$$\psi_{mn} = (\mathbb{I}_d \otimes U_{mn})\psi_d^+ \ , \tag{61}$$

where U_{mn} are unitary matrices defined as follows

$$U_{mn} e_k = \lambda^{mk} e_{k+n} \ , \tag{62}$$

with $\lambda = e^{2\pi i/d}$. The matrices U_{mn} define an orthonormal basis in the space $M_d(\mathbb{C})$ of complex $d \times d$ matrices. One easily shows

$$\mathrm{Tr}(U_{mn} U_{rs}^\dagger) = d\, \delta_{mr} \delta_{ns} \ . \tag{63}$$

Some authors [66] call U_{mn} generalized spin matrices since for $d = 2$ they reproduce standard Pauli matrices:

$$U_{00} = \mathbb{I}_2 \ , \ U_{01} = \sigma_1 \ , \ U_{10} = i\sigma_2 \ , \ U_{11} = \sigma_3 \ . \tag{64}$$

One calls a Hermitian operator W in $M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$ *Bell diagonal* if

$$W = \sum_{m,n=0}^{d-1} p_{mn} P_{mn} \ , \tag{65}$$

with $p_{mn} \in \mathbb{R}$, and

$$P_{mn} = |\psi_{mn}\rangle\langle\psi_{mn}| \ . \tag{66}$$

Example 4. Consider the flip operator in $d = 2$. One has

$$F = P_{00} + P_{10} + P_{01} - P_{11} \ , \tag{67}$$

which proves that F is Bell diagonal and possesses single negative eigenvalue.

Example 5. *Consider a family $W[a,b,c]$. One finds the following spectral representation*

$$W[a,b,c] = (a-2)P_{00} + (a+1)(P_{10} + P_{20}) + b\Pi_1 + c\Pi_2 \ , \tag{68}$$

where

$$\Pi_m = P_{0m} + P_{1m} + P_{2m} \ , \tag{69}$$

which shows that $W[a,b,c]$ is Bell diagonal with a single negative eigenvalue '$a-2$'.

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Example 6. Entanglement witness corresponding to the reduction map $\Lambda(X) = \mathbb{I}\mathrm{Tr}X - X$ in $M_d(\mathbb{C})$. One has

$$W = \frac{1}{d}\,\mathbb{I}_d \otimes \mathbb{I}_d - P_d^+ = \frac{1}{d}\sum_{k,l=0}^{d-1} P_{kl} - P_{00}\ , \tag{70}$$

which shows that W is Bell diagonal with a single negative eigenvalue $(1-d)/d$.

Corollary 1. *If $L < d$ and*

$$\lambda_\alpha^+ \geq \mu_1\ , \quad \alpha = L, \ldots, d^2 - 1\ , \tag{71}$$

with $\mu_1 = \frac{1}{d-L}\sum_{\alpha=0}^{L-1} |\lambda_\alpha^-|$, then $W = W_+ - W_-$ defines Bell diagonal entanglement witness.

8. Optimal maps in $M_{2k}(\mathbb{C})$

In this section we provide several examples of optimal indecomposable maps in $M_{2k}(\mathbb{C})$. Interestingly, some of them turn out to be extremal and even exposed [60, 61]. Consider $X \in M_{2k}(\mathbb{C}) = M_2(\mathbb{C}) \otimes M_k(\mathbb{C})$ represented as follows

$$X = \sum_{k,l=1}^{2} e_{kl} \otimes X_{kl}\ , \tag{72}$$

where $X_{kl} \in M_k(\mathbb{C})$. In what follows we shall use the following notation

$$X = \left(\begin{array}{c|c} X_{11} & X_{12} \\ \hline X_{21} & X_{22} \end{array}\right)\ , \tag{73}$$

to display the block structure of X. Robertson map [13] in $M_4(\mathbb{C})$ is defined as follows:

$$\Phi_4\left(\begin{array}{c|c} X_{11} & X_{12} \\ \hline X_{21} & X_{22} \end{array}\right) = \frac{1}{2}\left(\begin{array}{c|c} \mathbb{I}_2\,\mathrm{Tr}X_{22} & -[X_{12} + R_2(X_{21})] \\ \hline -[X_{21} + R_2(X_{12})] & \mathbb{I}_2\,\mathrm{Tr}X_{11} \end{array}\right)\ , \tag{74}$$

where R_2 is a reduction map in $M_2(\mathbb{C})$

$$R_2(X) = \mathbb{I}_2\mathrm{Tr}X - X\ . \tag{75}$$

Theorem 8. *Φ_4 defines positive indecomposable map. Moreover, it is extremal in the convex set of positive maps in $M_4(\mathbb{C})$.*

Interestingly

Theorem 9 ([61]). *Φ_4 is an exposed map.*

Following [35] and [34] one defines

$$\Phi_{2k}^{U}(X) = \frac{1}{2(k-1)}\left[R_n(X) - UX^T U^\dagger\right] , \tag{76}$$

where U is an antisymmetric unitary matrix in $M_{2k}(\mathbb{C})$. The above normalization guaranties that Φ_{2k}^{U} is unital. The characteristic feature of these maps is that for any rank-1 projector P its image under Φ_{2k}^{U} reads as follows:

$$\Phi_{2k}^{U}(P) = \frac{1}{2(k-1)}\left[\mathbb{I}_{2k} - P - Q\right] , \tag{77}$$

where $Q = UP^{\mathrm{T}}U^\dagger$ is a rank-1 projector orthogonal to P. Hence $\Phi_{2k}^{U}(P)$ is a projector which proves positivity of Φ_{2k}^{U}. Denote by U_0 the following “canonical" antisymmetric unitary matrix in $M_{2k}(\mathbb{C})$

$$U_0 = \mathbb{I}_k \otimes J , \tag{78}$$

where J is a symplectic matrix in $M_2(\mathbb{R})$, that is,

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{79}$$

Note, that if $V \in M_{2k}(\mathbb{R})$ is orthogonal then

$$U = VU_0V^{\mathrm{T}} , \tag{80}$$

is antisymmetric and unitary. Interestingly, the map Φ_{2k}^{0} corresponding to $U = U_0$ has the following block structure

$$\Phi_{2k}^{0}\left(\begin{array}{c|c|c|c} X_{11} & X_{12} & \cdots & X_{1k} \\ \hline X_{21} & X_{22} & \cdots & X_{2k} \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline X_{k1} & X_{k2} & \cdots & X_{kk} \end{array}\right) = \frac{1}{2(k-1)}\left(\begin{array}{c|c|c|c} A_1 & -B_{12} & \cdots & -B_{1k} \\ \hline -B_{21} & A_2 & \cdots & -B_{2k} \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline -B_{k1} & -B_{k2} & \cdots & A_k \end{array}\right) , \tag{81}$$

where

$$A_k = \mathbb{I}_2(\mathrm{Tr}X - \mathrm{Tr}X_{kk}) , \tag{82}$$

and

$$B_{kl} = X_{kl} - R_2(X_{lk}) , \tag{83}$$

and hence it reduces for $k = 2$ to the Robertson map (74).

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In the recent paper [44] we proposed another construction of maps in $M_{2k}(\mathbb{C})$. Now, instead of treating a $2k \times 2k$ matrix X as a $k \times k$ matrix with 2×2 blocks X_{ij} we consider alternative possibility, i.e. we consider X as a 2×2 with $k \times k$ blocks and define

$$\Psi_{2k}\left(\begin{array}{c|c} X_{11} & X_{12} \\ \hline X_{21} & X_{22} \end{array}\right) = \frac{1}{k}\left(\begin{array}{c|c} \mathbb{I}_k \,\mathrm{Tr} X_{22} & -[X_{12} + R_k(X_{21})] \\ \hline -[X_{21} + R_k(X_{12})] & \mathbb{I}_k \,\mathrm{Tr} X_{11} \end{array}\right) . \tag{84}$$

Again, normalization factor guaranties that the map is unital, i.e. $\Psi_{2k}(\mathbb{I}_2 \otimes \mathbb{I}_k) = \mathbb{I}_2 \otimes \mathbb{I}_k$. It is clear that for $k = 2$ one has $\Psi_4 = \Phi_4^0$.

Theorem 10 ([44]). Ψ_{2k} *defines a linear positive map in* $M_{2k}(\mathbb{C})$. *Moreover, it is an atomic and optimal map.*

In Ref. [51] we proposed the following generalization of the Robertson map Φ_{2k}: for any collection of $k(k-1)/2$ complex numbers z_{ij}, with $i < j$, satisfying $|z_{ij}| \leq 1$ we define $\Phi_{2k}^{(\mathbf{z})} : M_{2k}(\mathbb{C}) \longrightarrow M_{2k}(\mathbb{C})$ by

$$\Phi_{2k}^{(\mathbf{z})}\left(\begin{array}{c|c|c|c} X_{11} & X_{12} & \cdots & X_{1k} \\ \hline X_{21} & X_{22} & \cdots & X_{2k} \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline X_{k1} & X_{k2} & \cdots & X_{kk} \end{array}\right) = \frac{1}{2(k-1)}\left(\begin{array}{c|c|c|c} A_1 & -z_{12}B_{12} & \cdots & -z_{1k}B_{1k} \\ \hline -\bar{z}_{21}B_{21} & A_2 & \cdots & -z_{2k}B_{2k} \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline -\bar{z}_{k1}B_{k1} & -\bar{z}_{k2}B_{k2} & \cdots & A_k \end{array}\right) . \tag{85}$$

It is clear that form $z_{ij} = 1$ the map $\Phi_{2k}^{(\mathbf{z})}$ reduces to Φ_{2k}. One proves

Theorem 11 ([51]). $\Phi_{2k}^{(\mathbf{z})}$ *defines a positive map. Moreover,* $\Phi_{2k}^{(\mathbf{z})}$ *is optimal and indecomposable iff* $|z_{ij}| = 1$.

9. Conclusions

We provide characterization of several classes of positive maps in $M_d(\mathbb{C})$. Equivalently, due to the Choi-Jamiołkowski isomorphism, we characterized the corresponding classes of entanglement witnesses. Concerning the application in quantum entanglement theory the key role is played by indecomposable maps which can detect PPT entangled states. The presentation was illustrated with several examples of indecomposable positive maps/entanglement witnesses: the Choi-like maps in $M_3(\mathbb{C})$ and its generalizations in $M_d(\mathbb{C})$. It was shown that several maps from these families are optimal and even exposed. Similarly, the Robertson map in $M_4(\mathbb{C})$ and its generalizations in $M_{2k}(\mathbb{C})$ turn out to be optimal maps [original Robertson map is even exposed]. It should be stressed that there is no general method enabling one to construct all indecomposable positive maps and hence this subject deserves further studies.

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