

## An interpolation problem for completely positive maps on matrix algebras: solvability and parametrization

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We present certain existence criteria and parameterizations for an interpolation problem for completely positive maps that take given matrices from a finite set into prescribed matrices. Our approach uses density matrices associated to linear functionals on \*-subspaces of matrices, inspired by the Smith-Ward linear functional and Arveson's Hahn-Banach Type Theorem. A necessary and sufficient condition for the existence of solutions and a parametrization of the set of all solutions of the interpolation problem in terms of a closed and convex set of an affine space are obtained. Other linear affine restrictions, like trace preserving, can be included as well, hence covering applications to quantum channels that yield certain quantum states at prescribed quantum states. We also perform a careful investigation on the intricate relation between the positivity of the density matrix and the positivity of the corresponding linear functional.

**Keywords:** completely positive; interpolation; density matrix; Choi matrix; quantum channel

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### 1. Introduction

Letting  $M_n$  denote the unital  $C^*$ -algebra of all  $n \times n$  complex matrices, recall that a matrix  $A \in M_n$  is *positive semidefinite* if all its principal determinants are nonnegative. A linear map  $\varphi: M_n \rightarrow M_k$  is *completely positive* if, for all  $m \in \mathbb{N}$ , the linear map  $I_m \otimes \varphi: M_m \otimes M_n \rightarrow M_m \otimes M_k$  is *positive*, in the sense that it maps any positive semidefinite element from  $M_m \otimes M_n$  into a positive semidefinite element in  $M_m \otimes M_k$ . By  $CP(M_n, M_k)$  we denote the cone of all completely positive maps  $\varphi: M_n \rightarrow M_k$ . An equivalent notion, cf. Stinespring [1], is that of *positive semidefinite* map  $\varphi$ , that is, for all  $m \in \mathbb{N}$ , all  $h_1, \dots, h_m \in \mathbb{C}^n$ , and all  $A_1, \dots, A_m \in M_n$ , we have

$$\sum_{i,j=1}^m \langle \varphi(A_j^* A_i) h_j, h_i \rangle \geq 0. \quad (1.1)$$

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In this article, we consider the following

**Interpolation Problem** Given matrices  $A_v \in M_n$  and  $B_v \in M_k$  for  $v = 1, \dots, N$ , determine  $\varphi \in \text{CP}(M_n, M_k)$  subject to the conditions

$$\varphi(A_v) = B_v, \text{ for all } v = 1, \dots, N. \tag{1.2}$$

The meaning of ‘determine’ is rather vague so we have to make it clear: firstly, one should find necessary and/or sufficient conditions for the existence of such a solution  $\varphi$ , secondly, one should find an explicit parametrization of all solutions and, lastly, but not the least, one should find techniques (numerical, computational, etc.) to determine (approximate) solutions. Other conditions like trace preserving may be required as well, with direct applications to quantum information theory. In this general formulation, the interpolation problem has been considered by Li and Poon in [2], where solutions have been obtained in case when the given input and output data are Hermitian matrices that mutually commute, respectively. The purpose of this article is to approach, from a general perspective, existence criteria and parametrization of solutions of the interpolation problem. The solvability of the interpolation problem is characterized in Theorem 3.3 from which an explicit parametrization of the set of all solutions in terms of a closed and convex set of an affine space follows.

A more concrete motivation for considering the interpolation problem is provided by the concept of ‘quantum operation’, cf. Kraus [3] and [4], in the more modern terminology, a *quantum channel*, that is, a completely positive linear map that is trace preserving. A natural question related to these mathematical objects refers to finding a quantum channel that can take certain given quantum states from a finite list into some other prescribed quantum states, which is a special case of interpolation problem. In this respect, Alberti and Uhlmann [5] find a necessary and sufficient condition for a pair of qubits (quantum states in  $M_2$ ) to be mapped under the action of a quantum channel onto another given pair of qubits. For larger sets of pure states, the problem has been considered from many other perspectives, see Chefles et al. [6] and the bibliography cited there. More general criteria for existence of solutions have been considered by Huang et al. in [7], while Heinosaari et al. obtain in [8] other criteria of existence of solutions as well as techniques to approximate solutions in terms of semidefinite programming, in the sense of Nesterov and Nemirovsky [9] and Vanderberghe and Boyd [10].

Another motivation for considering the interpolation problem comes from quantum tomography, e.g. see Chuang and Nielsen [11], which requires the explicit calculation of the quantum channel at each matrix unit. On the other hand, it is more realistic to assume that incomplete data may be available only and that the input data may not be related to matrix units at all, e.g. see D’Ariano and Lo Presti [12] and Gonçalves et al. [13].

In order to briefly describe our approach and results, let us denote  $\mathbf{A} = (A_1, \dots, A_N)$  and call it the *input data* and, similarly,  $\mathbf{B} = (B_1, \dots, B_N)$  and call it the *output data*, as well as

$$\mathcal{C}_{\mathbf{A}, \mathbf{B}} := \{\varphi \in \text{CP}(M_n, M_k) \mid \varphi(A_v) = B_v, \text{ for all } v = 1, \dots, N\}. \tag{1.3}$$

Clearly, the set  $\mathcal{C}_{\mathbf{A}, \mathbf{B}}$  is convex and closed, but it may or may not be compact. Since the maps  $\varphi \in \text{CP}(M_n, M_k)$  are, by definition, linear, without loss of generality one can assume that the set  $\{A_1, \dots, A_N\}$  is linearly independent, otherwise some linear dependence conditions on the output data  $\mathbf{B}$  are necessary. On the other hand, since any  $\varphi \in \text{CP}(M_n, M_k)$  is Hermitian, in the sense that  $\varphi(A^*) = \varphi(A)^*$  for all  $A \in M_n$ , it follows that, without loss of generality,

one can assume that all matrices  $A_1, \dots, A_N, B_1, \dots, B_N$  are Hermitian. In particular, letting  $\mathcal{S}_A$  denote the linear span of  $A_1, \dots, A_N$ , it follows that  $\mathcal{S}_A$  is a  $*$ -subspace of  $M_n$ , that is, it is a linear subspace stable under taking adjoints, and then, letting  $\varphi_{A,B}: \mathcal{S}_A \rightarrow M_k$  be the linear map uniquely determined by the conditions

$$\varphi_{A,B}(A_\nu) = B_\nu, \quad \nu = 1, \dots, N,$$

it follows that any  $\varphi \in \text{CP}(M_n, M_k)$  satisfying the constraints (1.2) should necessarily be an extension of  $\varphi_{A,B}$ . Inspired by Smith and Ward [14], to  $\varphi_{A,B}$  we associate a linear functional  $s_{A,B}$ , see (3.4), and call it the Smith-Ward linear functional, and then we go further and we associate a ‘density matrix’  $D_{A,B} \in M_k \otimes \mathcal{S}_A$  by  $s_{A,B}(C) = \text{tr}(D_{A,B}^* C)$  for all  $C \in M_k \otimes \mathcal{S}_A$ . In Theorem 3.3, we show that the solvability of the interpolation problem is equivalent to the fact that the affine subspace  $D_{A,B} + M_k \otimes \mathcal{S}_A^\perp$  contains positive semidefinite matrices. Consequently, a parametrization of the set of all solutions of the interpolation problem by the closed convex subset  $\mathcal{P}_{A,B} := \{P \in (M_k \otimes \mathcal{S}_A^\perp)^h \mid P \geq -D_{A,B}\}$  is obtained through an affine isomorphism. In Section 3.2 we show that, if the input data  $A$  are orthonormalized with respect to the Hilbert-Schmidt inner product, then the density matrix is easily calculable as  $D_{A,B} = \sum_{\nu=1}^N B_\nu^T \otimes A_\nu$  and this considerably simplifies the criterion of solvability of the interpolation problem, see Theorem 3.12. Also, we observe that the Gram-Schmidt orthonormalization does not affect the other assumptions.

If the  $*$ -subspace  $\mathcal{S}_A$  contains the identity matrix  $I_n$  (e.g. if we are interested in solutions  $\varphi$  that are unital, that is,  $\varphi(I_n) = I_k$ ), making it an *operator system*, [15] then  $\mathcal{S}_A$  is linearly generated by the cone of its positive semidefinite matrices  $\mathcal{S}_A^+$ . In this case, there is the celebrated Arveson’s Hahn-Banach Type Theorem [16] and Smith-Ward’s proof, [14] see Theorem 2.6, that can be used, see Theorem 3.6, in order to show that the solvability of the Interpolation Problem is equivalent with two other assertions: firstly, with the complete positivity of  $\varphi_{A,B}$  and, secondly, with the positivity of  $s_{A,B}$ .

In order to compare our results with the above-mentioned articles, let us note that our solution as in Theorem 3.3 shows that the interpolation problem is a semidefinite programming problem, a fact already observed in [8] and [13], but our characterization in terms of  $D_{A,B} + M_k \otimes \mathcal{S}_A^\perp$  puts the interpolation problem in the dual form of a semidefinite programming problem, cf. [9,10], which makes it different from all previous works.

It is a simple observation, see Remarks 3.5, that the positive semidefiniteness of the density matrix  $D_{A,B}$  is sufficient for the existence of solutions to the interpolation problem but, in general, this is not a necessary condition. We perform a careful investigation on this issue in Section 2.4 and we provide examples and counter-examples illustrating the complexity of this phenomenon. In addition, in Theorem 4.3, we show that in case a  $*$ -subspace  $\mathcal{S}$  is generated by matrix units and also generated by  $\mathcal{S}^+$ , then the density matrix of any positive linear functional on  $\mathcal{S}$  is positive semidefinite if and only if  $\mathcal{S}$  is an algebra. Therefore, in this special case, it is necessary to impose the additional assumption that the  $*$ -subspace  $\mathcal{S}_A$  is an algebra, in order for the solvability of the interpolation problem to be equivalent to the positive definiteness of  $D_{A,B}$ . However, exotic cases of  $*$ -subspaces that are not algebras but when this equivalence happens may occur as well, see Examples 2.9.

Another observation on the density matrix  $D_{A,B}$  is that, one might think that it is the Choi matrix [17] that plays the major role in getting criteria of existence of solutions of the interpolation problem, but this seems not to be the case: firstly, in order to define the Choi matrix, see Section 2.1, we have to use all the matrix units, but the subspace  $\mathcal{S}_A$

might not contain any of them and, secondly, the Choi matrix does not relate well with the ‘action’ of the linear map that it represents, while the density matrix does. Actually, once we explicitly show the relation between the density matrix and the Choi matrix of a given map  $\varphi \in \text{CP}(M_n, M_k)$ , see Proposition 4.1, we can define a ‘partial Choi matrix’, see (4.5), for linear maps on subspaces.

In Section 3.3 we consider the interpolation problem for a single interpolation pair, that is,  $N = 1$ , consisting of Hermitian matrices. By using techniques from indefinite inner product spaces, e.g. see [18], we derive criteria of existence of solutions of the interpolation problem with only one operation element, get a necessary and sufficient condition of solvability in terms of the definiteness characteristics of the data, and estimate the minimal number of the operation elements of the solutions.

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## 2. Notation and preliminary results

### 2.1. The Choi matrix and the Kraus form

Following [19],  $n \in \mathbb{N}$  let  $\{e_i^{(n)}\}_{i=1}^n$  be the canonical basis of  $\mathbb{C}^n$ . The space  $M_{n,k}$  of  $n \times k$  matrices is identified with  $\mathcal{B}(\mathbb{C}^k, \mathbb{C}^n)$ , the vector space of all linear transformations  $\mathbb{C}^k \rightarrow \mathbb{C}^n$ . For  $n, k \in \mathbb{N}$  we consider the matrix units  $\{E_{l,i}^{(n,k)} \mid l = 1, \dots, n, i = 1, \dots, k\} \subset M_{n,k}$  of size  $n \times k$ , that is,  $E_{l,i}^{(n,k)}$  is the  $n \times k$  matrix with all entries 0 except the  $(l, i)$ -th entry which is 1. In case  $n = k$ , we denote simply  $E_{l,i}^{(n)} = E_{l,i}^{(n,n)}$ . Recall that  $M_n$  is organized as a  $C^*$ -algebra in a natural way and hence, positive elements, that is, positive semidefinite matrices in  $M_n$ , are well defined.

Given a linear map  $\varphi: M_n \rightarrow M_k$  define an  $kn \times kn$  matrix  $\Phi_\varphi$  by

$$\Phi_\varphi = \left[ \varphi \left( E_{l,m}^{(n)} \right) \right]_{l,m=1}^n. \tag{2.1}$$

This transformation appears more or less explicitly at de Pillis [20], Jamiołkowski [21], Hill [22], and Choi [17]. In the following, we describe more explicitly the transformation  $\varphi \mapsto \Phi_\varphi$ . We use the lexicographic reindexing of  $\{E_{l,i}^{(n,k)} \mid l = 1, \dots, n, i = 1, \dots, k\}$ , more precisely

$$\left( E_{1,1}^{(n,k)}, \dots, E_{1,k}^{(n,k)}, E_{2,1}^{(n,k)}, \dots, E_{2,k}^{(n,k)}, \dots, E_{n,1}^{(n,k)}, \dots, E_{n,k}^{(n,k)} \right) = (\mathcal{E}_1, \mathcal{E}_2, \dots, \mathcal{E}_{nk}) \tag{2.2}$$

An even more explicit form of this reindexing is the following

$$\mathcal{E}_r = E_{l,i}^{(n,k)} \text{ where } r = (l - 1)k + i, \quad \text{for all } l = 1, \dots, n, i = 1, \dots, k. \tag{2.3}$$

The formula

$$\varphi_{(l-1)k+i,(m-1)k+j} = \left\langle \varphi \left( E_{l,m}^{(n)} e_j^{(k)}, e_i^{(k)} \right) \right\rangle, \quad i, j = 1, \dots, k, \quad l, m = 1, \dots, n, \quad (2.4)$$

and its inverse

$$\varphi(C) = \sum_{r,s=1}^{nk} \varphi_{r,s} \mathcal{E}_r^* C \mathcal{E}_s, \quad C \in M_n, \quad (2.5)$$

establish a linear and bijective correspondence

$$\mathcal{B}(M_n, M_k) \ni \varphi \mapsto \Phi_\varphi = [\varphi_{r,s}]_{r,s=1}^{nk} \in M_{nk}. \quad (2.6)$$

The formulae (2.4) and its inverse (2.5) establish an affine and order preserving isomorphism

$$\text{CP}(M_n, M_k) \ni \varphi \mapsto \Phi_\varphi \in M_{nk}^+. \quad (2.7)$$

Given  $\varphi \in \mathcal{B}(M_n, M_k)$  the matrix  $\Phi_\varphi$  as in (2.1) is called *the Choi matrix* of  $\varphi$ .

Let  $\varphi : M_n \rightarrow M_k$  be a completely positive map. Then, cf. Kraus [3] and Choi [17], there are  $n \times k$  matrices  $V_1, V_2, \dots, V_m$  with  $m \leq nk$  such that

$$\varphi(A) = V_1^* A V_1 + V_2^* A V_2 + \dots + V_m^* A V_m \text{ for all } A \in M_n. \quad (2.8)$$

The representation (2.8) is called the *Kraus representation* of  $\varphi$  and the matrices  $V_1, \dots, V_m$  are called the *operation elements*. Note that the representation (2.8) of a given completely positive map  $\varphi$  is highly nonunique, not only with respect to its operation elements but also with respect to  $m$ , the number of these elements. The minimal number of the operation elements in the Kraus form representation of a completely positive map  $\varphi \in \text{CP}(M_n, M_k)$  with Choi matrix  $\Phi$  is  $\text{rank}(\Phi)$ .

### 2.2. \*-Subspaces

For a fixed natural number  $m$ ,  $\mathcal{S} \subseteq M_m$  is called a *\*-subspace* if it is a linear subspace of  $M_m$  that is stable under taking adjoints, that is,  $A^* \in \mathcal{S}$  for any  $A \in \mathcal{S}$ . Note that, both the real part and imaginary part of matrices in  $\mathcal{S}$  are in  $\mathcal{S}$  and hence  $\mathcal{S}$  is linearly generated by the real subspace  $\mathcal{S}^h$  of all its Hermitian matrices. Also,  $\mathcal{S}^+ = \{A \in \mathcal{S} \mid A \geq 0\}$  is a cone in  $\mathcal{S}^h$  but, in general,  $\mathcal{S}^+$  may fail to linearly generate  $\mathcal{S}^h$ . Recall [15] that a *\*-subspace*  $\mathcal{S}$  in  $M_m$  is called an *operator system* if the identity matrix  $I_m \in \mathcal{S}$ . Any operator system  $\mathcal{S}$  is linearly generated by  $\mathcal{S}^+$ , e.g. observing that any Hermitian matrix  $B \in \mathcal{S}$  can be written

$$B = \frac{1}{2}(\|B\|I_m + B) - \frac{1}{2}(\|B\|I_m - B),$$

hence a difference of two positive semidefinite matrices in  $\mathcal{S}$ . The next proposition provides different characterizations of those *\*-subspaces*  $\mathcal{S}$  of matrices that are linearly generated by  $\mathcal{S}^+$ , as well as a model that points out the distinguished role of operator systems. We need first to recall a technical lemma.

LEMMA 2.1 *Given two matrices  $A, B \in M_m^+$ , we have  $B \leq \alpha A$ , for some  $\alpha > 0$ , if and only if  $\text{Ran}(B) \subseteq \text{Ran}(A)$ .*

*Proof* A folklore result in operator theory, e.g. see [23], says that for two matrices  $A, B \in M_m$ , the inequality  $BB^* \leq \alpha AA^*$ , for some  $\alpha > 0$ , is equivalent with  $\text{Ran}(B) \subseteq \text{Ran}(A)$ .

Consequently, if  $A, B \in M_m^+$  then  $B \leq A$  if and only if  $\text{Ran}(B^{1/2}) \subseteq \text{Ran}(A^{1/2})$ . From here the statement follows since we have  $\text{Ran}(P) = \text{Ran}(P^{1/2})$  for any positive semidefinite matrix  $P$ .  $\square$

PROPOSITION 2.2 *Let  $\mathcal{S}$  be a  $*$ -space in  $M_m$ . The following assertions are equivalent:*

- (i)  $\mathcal{S}$  is linearly generated by  $\mathcal{S}^+$ .
- (ii) There exists  $A \in \mathcal{S}^+$  such that for any  $B \in \mathcal{S}^h$  we have  $B \leq \alpha A$  for some  $\alpha > 0$ .
- (iii) For any  $B \in \mathcal{S}^h$  there exists  $A \in \mathcal{S}^+$  with  $B \leq A$ .
- (iv) There exists  $T \in M_m$  a matrix of rank  $r$ , with  $\text{Ran}(T) = \mathbb{C}^r \oplus 0 \subseteq \mathbb{C}^m$ , and an operator system  $\mathcal{T} \subseteq M_r$  such that

$$S = T^*(\mathcal{T} \oplus 0_{m-r})T, \tag{2.9}$$

where  $0_{m-r}$  denotes the  $(m - r) \times (m - r)$  null matrix.

*Proof*

(i) $\Rightarrow$ (ii). Assuming that  $\mathcal{S}$  is linearly generated by  $\mathcal{S}^+$ , let  $A$  be a matrix in  $\mathcal{S}^+$  of maximal rank. We first show that, for any  $B \in \mathcal{S}^+$  we have  $B \leq \alpha A$  for some  $\alpha > 0$ . To this end, assume that this is not true hence, by Lemma 2.1,  $\text{Ran}(B) \not\subseteq \text{Ran}(A)$  hence,  $\text{Ran}(A)$  is a proper subspace of  $\text{Ran}(A) + \text{Ran}(B)$ . Since  $A, B \leq A + B$ , again by Lemma 2.1 it follows  $\text{Ran}(B) + \text{Ran}(A) \subseteq \text{Ran}(A + B)$ . But then,  $A + B \in \mathcal{S}^+$  has bigger rank than  $A$ , which contradicts the choice of  $A$ .

Let now  $B \in \mathcal{S}^h$  be arbitrary. By assumption,  $B = B_1 - B_2$  with  $B_j \in \mathcal{S}^+$  for  $j = 1, 2$  hence, by what has been proven before, there exist  $\alpha > 0$  such that  $B_1 \leq \alpha A$ , hence  $B \leq B_1 \leq \alpha A$ .

(ii) $\Rightarrow$ (iii). This implication is obvious.

(iii) $\Rightarrow$ (i). Since  $\mathcal{S}$  is a  $*$ -subspace, in order to prove that  $\mathcal{S}$  is linearly generated by  $\mathcal{S}^+$ , it is sufficient to prove that  $\mathcal{S}^h$  is (real) linearly generated by  $\mathcal{S}^+$ . To see this, let  $B \in \mathcal{S}^h$  be arbitrary. By assumption, there exist  $A_j \in \mathcal{S}^+$ ,  $j = 1, 2$ , such that  $B \leq A_1$  and  $-B \leq A_2$  hence, letting  $A = A_1 + A_2 \in \mathcal{S}^+$ , we have

$$B = \frac{1}{2}(A - B) - \frac{1}{2}(A + B),$$

where  $A - B, A + B \in \mathcal{S}^+$ .

(ii) $\Rightarrow$ (iv). Let  $A \in \mathcal{S}^+$  be a matrix having the property that for any  $B \in \mathcal{S}^h$  there exists  $\alpha > 0$  such that  $B \leq \alpha A$ . By Lemma 2.1, it follows that for any  $B \in \mathcal{S}^+$  we have  $\text{Ran}(B) \subseteq \text{Ran}(A)$  hence, since  $\mathcal{S}$  is linearly generated by  $\mathcal{S}^+$ , it follows that for any  $B \in \mathcal{S}$  we have  $\text{Ran}(B) \subseteq \text{Ran}(A)$ , in particular,  $\text{Ran}(A)$  reduces  $B$  and

$$B = \begin{bmatrix} B_0 & 0 \\ 0 & 0 \end{bmatrix}, \quad \text{w. r. t. } \mathbb{C}^m = \text{Ran}(A) \oplus \ker(A).$$

Letting  $r$  denote the rank of  $A$ , observe now that  $A_0$  is positive semidefinite and invertible as a linear transformation in  $\text{Ran}(A)$ , hence

$$\mathcal{T}_0 = \{A_0^{-1/2} B_0 A_0^{-1/2} \mid B \in \mathcal{S}\}$$

is an operator system in  $\mathcal{B}(\text{Ran}(A))$ . Then consider a unitary transformation  $V$  in  $M_m$  such that it maps  $\text{Ran}(A)$  to  $\mathbb{C}^r$  and  $\ker(A)$  to  $\mathbb{C}^{m-r}$ , letting

$$\mathcal{T} = V\mathcal{T}_0V^* \text{ and } T = VA^{1/2}$$

the conclusion follows.

(iv) $\Rightarrow$ (i). This implication is clear. □

**COROLLARY 2.3** *If the  $*$ -subspace  $\mathcal{S}$  of  $M_m$  contains a positive definite matrix, then  $\mathcal{S}$  is linearly generated by  $\mathcal{S}^+$ .*

*Proof* Indeed, if  $P \in \mathcal{S}$  is positive definite, then  $\mathcal{T} = P^{-1/2}\mathcal{S}P^{-1/2}$  is an operator system and then  $\mathcal{S} = P^{1/2}\mathcal{T}P^{1/2}$  is linearly generated by  $\mathcal{S}^+$ . □

In the following, we will use a particular case of the celebrated theorem of Kantorovich [24], see also Theorem I.30 in [25], of Hahn-Banach type.

**LEMMA 2.4** *Let  $\mathcal{S}$  be a  $*$ -subspace of  $M_m$  that is linearly generated by  $\mathcal{S}^+$ , and let  $f: \mathcal{S} \rightarrow \mathbb{C}$  be a positive linear map, in the sense that it maps any element  $A \in \mathcal{S}^+$  to a nonnegative number  $f(A)$ . Then, there exists a positive linear functional  $\tilde{f}: M_m \rightarrow \mathbb{C}$  that extends  $f$ .*

*Proof* Briefly, the idea is to consider the  $\mathbb{R}$ -linear functional  $f_h = f|_{\mathcal{S}^h}$  and note that  $f_h$  is positive. By Proposition 2.2, there exists  $A \in \mathcal{S}^+$  such that for all  $B \in \mathcal{S}^h$  there exists  $\alpha > 0$  with  $B \leq \alpha A$ . By Lemma 2.1, we have  $\text{Ran}(B) \subseteq \text{Ran}(A)$  for all  $B \in \mathcal{S}^h$ . Let  $p: \mathcal{B}(\text{Ran}(A))^h \rightarrow \mathbb{R}$  be defined by

$$p(C) = \inf \{f_h(B) \mid C \leq B \in \mathcal{S}^h\}, \quad C \in \mathcal{B}(\text{Ran}(A))^h. \tag{2.10}$$

Then  $p$  is a sublinear functional on the  $\mathbb{R}$ -linear space  $\mathcal{B}(\text{Ran}(A))^h$  and  $f(B) = p(B)$  for all  $B \in \mathcal{S}^h$ . By the Hahn-Banach Theorem, there exists a linear functional  $g: \mathcal{B}(\text{Ran}(A))^h \rightarrow \mathbb{R}$  that extends  $f_h$  and such that  $g(B) \leq p(B)$  for all  $B \in \mathcal{B}(\text{Ran}(A))^h$ . Then, for any  $B \in M_m^+$ , since  $-B \leq 0$  it follows  $-g(B) = g(-B) \leq p(-B) \leq f_h(0) = 0$ , hence  $g(B) \geq 0$ . Then, let  $\tilde{f}$  be the canonical extension of  $g$  to  $\mathcal{B}(\text{Ran}(A)) = \mathcal{B}(\text{Ran}(A))^h + i\mathcal{B}(\text{Ran}(A))^h$ , in the usual way, and finally extend  $\tilde{f}$  to  $M_m$  by letting  $\tilde{f}(B) = \tilde{f}(P_{\text{Ran}(A)}B|_{\text{Ran}(A)})$  for all  $B \in M_m$ , where  $P_{\text{Ran}(A)}$  denotes the orthogonal projection of  $\mathbb{C}^m$  onto  $\text{Ran}(A)$ . □

We will also need the following

**LEMMA 2.5** *Let  $\mathcal{S}$  be a  $*$ -subspace in  $M_n$  and let  $\mathcal{S}^\perp$  be the orthogonal complement space associated to  $\mathcal{S}$  with respect to the Hilbert-Schmidt inner product*

$$\mathcal{S}^\perp = \{E \in M_n \mid \text{tr}(C^*E) = 0, \text{ for all } C \in \mathcal{S}\}. \tag{2.11}$$

Then:

- (a)  $\mathcal{S}^\perp$  is a  $*$ -subspace of  $M_n$ , hence linearly generated by its Hermitian matrices.
- (b)  $(M_k \otimes \mathcal{S})^\perp = M_k \otimes \mathcal{S}^\perp$ , in particular,  $(M_k \otimes \mathcal{S})^\perp$  is a  $*$ -subspace of  $M_k \otimes M_n$ .
- (c) If  $\mathcal{S}$  is an operator system then any matrix  $C \in \mathcal{S}^\perp$  has zero trace, in particular  $\mathcal{S}^\perp \cap M_n^+ = \{0\}$ .



- (d) If  $\mathcal{S}$  is an operator system then any matrix in  $(M_k \otimes \mathcal{S})^\perp$  has zero trace, hence  $(M_k \otimes \mathcal{S})^\perp$  does not contain nontrivial positive semidefinite matrices.

*Proof*

- (a) Clearly,  $\mathcal{S}^\perp$  is a subspace of  $M_n$ . Let  $E \in \mathcal{S}^\perp$ , hence  $\text{tr}(E^*C) = 0$  for all  $C \in \mathcal{S}$ . Then,  $0 = \text{tr}(E^*C) = \text{tr}(C^*E) = \text{tr}(EC^*) = \text{tr}((E^*)^*C^*)$  for all  $C \in \mathcal{S}$  and, since  $\mathcal{S}$  is stable under taking adjoints, this implies that  $E^* \in \mathcal{S}^\perp$ .
- (b) A moment of thought shows that  $M_k \otimes \mathcal{S}^\perp \subseteq (M_k \otimes \mathcal{S})^\perp$ . On the other hand,  $\dim((M_k \otimes \mathcal{S})^\perp) = k^2n^2 - k^2 \dim(\mathcal{S}) = k^2(n^2 - \dim(\mathcal{S})) = \dim(M_k \otimes \mathcal{S}^\perp)$ , hence the desired conclusion follows.
- (c) This is a consequence of the fact that  $I_n \in \mathcal{S}$  and the fact that the trace is faithful.
- (d) This is a consequence of the statements (b) and (c).  $\square$

### 2.3. The Smith-Ward functional

In the following, we first recall a technical concept introduced by Smith and Ward, cf. the proof of Theorem 2.1 in [14], and there used to provide another proof to the Arveson’s Hahn-Banach Theorem [16] for completely positive maps, see also Chapter 6 in [15]. Consider  $\mathcal{S}$  a subspace of  $M_n$ . Note that, for any  $k \in \mathbb{N}$ ,  $M_k(\mathcal{S})$ , the collection of all  $k \times k$  block-matrices with entries in  $\mathcal{S}$ , canonically identified with  $M_k \otimes \mathcal{S}$ , is embedded into the  $C^*$ -algebra  $M_k(M_n) = M_k \otimes M_n$  and hence it inherits a natural order relation, in particular, positivity of its elements is well defined. If  $\mathcal{S}$  is a  $*$ -subspace then  $M_k(\mathcal{S})$  is a  $*$ -subspace as well and if, in addition, the  $*$ -subspace  $\mathcal{S}$  is linearly generated by the cone of its positive semidefinite matrices, the same is true for  $M_k(\mathcal{S})$ , e.g. by Proposition 2.2. A linear map  $\varphi: \mathcal{S} \rightarrow M_k$ , is called *positive* if it maps any positive semidefinite matrix from  $\mathcal{S}$  to a positive semidefinite matrix in  $M_k$ . Moreover, for  $m \in \mathbb{N}$ , letting  $\varphi_m = I_m \otimes \varphi: M_m \otimes \mathcal{S} \rightarrow M_m \otimes M_k$ , by means of the canonical identification of  $M_m \otimes \mathcal{S}$  with  $M_m(\mathcal{S})$ , the  $C^*$ -algebra of all  $m \times m$  block-matrices with entries elements from  $\mathcal{S}$ , it follows that

$$\varphi_m \left( [a_{i,j}]_{i,j=1}^m \right) = [\varphi(a_{i,j})]_{i,j=1}^m, \quad [a_{i,j}]_{i,j=1}^m \in M_m(\mathcal{S}).$$

Then,  $\varphi$  is called *m-positive* if  $\varphi_m$  is a positive map, and it is called *completely positive* if it is *m-positive* for all  $m \in \mathbb{N}$ . However, positive semidefiniteness in the sense of (1.1) cannot be defined, at this level of generality.

To any linear map  $\varphi: \mathcal{S} \rightarrow M_k$ , where  $\mathcal{S} \subseteq M_n$  is some linear subspace, one associates a linear functional  $s_\varphi: M_k(\mathcal{S}) \rightarrow \mathbb{C}$ , via the canonical identification of  $M_k(\mathcal{S}) \simeq M_k \otimes \mathcal{S}$ , by

$$\begin{aligned} s_\varphi \left( [A_{i,j}]_{i,j=1}^k \right) &= \sum_{i,j=1}^k \left\langle \varphi(A_{i,j}) e_j^{(k)}, e_i^{(k)} \right\rangle_{\mathbb{C}^k} \\ &= \left\langle \left( I_k \otimes \varphi \left( [A_{i,j}]_{i,j=1}^k \right) \right) e^{(k)}, e^{(k)} \right\rangle_{\mathbb{C}^{k^2}} \\ &= \left\langle [\varphi(A_{i,j})]_{i,j=1}^k e^{(k)}, e^{(k)} \right\rangle_{\mathbb{C}^{k^2}} \end{aligned} \tag{2.12}$$



where  $[A_{i,j}]_{i,j=1}^k \in M_k(\mathcal{S})$ , that is, it is a  $k \times k$  block-matrix, in which each block  $A_{i,j}$  is an  $n \times n$  matrix from  $\mathcal{S}$ , and  $e^{(k)}$  is defined by

$$e^{(k)} = e_1^{(k)} \oplus \dots \oplus e_k^{(k)} \in \mathbb{C}^{k^2} = \mathbb{C}^k \oplus \dots \oplus \mathbb{C}^k. \tag{2.13}$$

The formula (2.12) establishes a linear isomorphism

$$\mathcal{B}(\mathcal{S}, M_k) \ni \varphi \mapsto s_\varphi \in (M_k \otimes \mathcal{S})^* \simeq \mathcal{B}(M_k \otimes \mathcal{S}, \mathbb{C}), \tag{2.14}$$

with the inverse transformation

$$(M_k \otimes \mathcal{S})^* \simeq \mathcal{B}(M_k \otimes \mathcal{S}, \mathbb{C}) \ni s \mapsto \varphi_s \in \mathcal{B}(\mathcal{S}, M_k) \tag{2.15}$$

given by the formula

$$\varphi_s(A) = \left[ s \left( E_{i,j}^{(k)} \otimes A \right) \right]_{i,j=1}^k, \quad A \in \mathcal{S}. \tag{2.16}$$

The importance of the Smith-Ward functional relies on the facts gathered in the following theorem: the equivalence of (a) and (d) is a particular case of the Arveson’s Hahn-Banach Theorem,[16] while the equivalence of (a), (b) and (c) is essentially due to Smith and Ward [14] as a different proof of Arveson’s result.

**THEOREM 2.6** *Let  $\mathcal{S}$  be a  $*$ -subspace of  $M_n$  that is linearly generated by  $\mathcal{S}^+$  and let  $\varphi: \mathcal{S} \rightarrow M_k$  be a linear map. The following assertions are equivalent:*

- (a)  $\varphi$  is completely positive.
- (b)  $\varphi$  is  $k$ -positive.
- (c)  $s_\varphi$  is a positive functional.
- (d) There exists  $\tilde{\varphi} \in \text{CP}(M_k, M_n)$  that extends  $\varphi$ .

*Proof* Clearly (a) implies (b), the fact that (b) implies (c) follows from the definition of  $s_\varphi$  as in (2.12), while (d) implies (a) is clear as well. The only nontrivial part is (c) implies (d). Briefly, following the proofs of Theorems 6.1 and 6.2 in [15], the idea is to use Kantorovich’s Theorem as in Lemma 2.4 in order to extend  $s_\varphi$  to a positive functional  $\tilde{s}$  on  $M_k \otimes M_n \simeq M_k(M_n) \simeq M_{kn}$  then, in view of (2.16), let  $\tilde{\varphi}: M_k \rightarrow M_n$  be defined by

$$\tilde{\varphi}(A) = \left[ \tilde{s} \left( E_{i,j}^{(k)} \otimes A \right) \right]_{i,j=1}^k, \quad A \in M_n, \tag{2.17}$$

and note that  $\tilde{\varphi}$  extends  $\varphi$ . Finally, in order to prove that  $\tilde{\varphi}$  is completely positive it is sufficient to prove that it is positive semidefinite, see (1.1). To see this, let  $m \in \mathbb{N}$ ,  $A_1, \dots, A_m \in M_n$ , and  $h_1, \dots, h_m \in \mathbb{C}^k$  be arbitrary. Then, letting

$$h_j = \sum_{l=1}^k \lambda_{i,l} e_l^{(k)}, \quad j = 1, \dots, m,$$

we have

$$\begin{aligned} \sum_{i,j=1}^m \langle \tilde{\varphi}(A_i^* A_j) h_j, h_i \rangle_{\mathbb{C}^k} &= \sum_{i,j=1}^m \sum_{l,p=1}^k \lambda_{j,l} \bar{\lambda}_{i,p} \langle \tilde{\varphi}(A_i^* A_j) e_l^{(k)}, e_p^{(k)} \rangle_{\mathbb{C}^k} \\ &= \sum_{i,j=1}^m \sum_{l,p=1}^k \lambda_{j,l} \bar{\lambda}_{i,p} \tilde{s} \left( A_i^* A_j \otimes E_{p,l}^{(k)} \right) \end{aligned}$$

then, for each  $i=1, \dots, m$ , letting  $B_i$  denote the  $k \times k$  matrix whose first row is  $\lambda_{i,1}, \dots, \lambda_{i,k}$  and all the others are 0, hence  $B_i^* B_j = \sum_{l,p=1}^k \lambda_{j,l} \bar{\lambda}_{i,p} E_{p,l}^{(k)}$ , we have

$$\begin{aligned} &= \sum_{i,j=1}^m \tilde{s}(A_i^* A_j \otimes B_i^* B_j) \\ &= \tilde{s} \left( \left( \sum_{i=1}^m A_i \otimes B_i \right)^* \left( \sum_{j=1}^m A_j \otimes B_j \right) \right) \geq 0. \end{aligned}$$

□

Actually, from the proof of Theorem 2.6, it is easy to observe that (2.12) and (2.16) establish an affine and order preserving bijection between the cone  $\text{CP}(\mathcal{S}, M_k)$  and the cone  $\{s: M_k(\mathcal{S}) \rightarrow \mathbb{C} \mid s \text{ linear and positive}\}$ .

### 2.4. The density matrix

We consider  $M_m$  as a Hilbert space with the Hilbert-Schmidt inner product, that is,  $\langle C, D \rangle_{\text{HS}} = \text{tr}(D^* C)$ , for all  $C, D \in M_m$ . To any linear functional  $s: M_m \rightarrow \mathbb{C}$ , by the representation theorem for (bounded) linear functionals on a Hilbert space, in our case  $M_m$  with the Hilbert-Schmidt inner product, one associates uniquely a matrix  $D_s \in M_m$ , such that

$$s(C) = \text{tr}(D_s^* C), \quad C \in M_m. \tag{2.18}$$

Clearly,  $s \mapsto D_s$  is a conjugate linear bijection between the dual space of  $M_m$  and  $M_m$ .

*Remark 2.7* Using the properties of the trace, it follows that  $s$  is a positive functional if and only if the matrix  $D_s$  is positive semidefinite. Indeed, if  $D_s$  is positive semidefinite, then for all positive semidefinite matrix in  $M_m$ , we have  $\text{tr}(D_s C) = \text{tr}(C^{1/2} D_s C^{1/2}) \geq 0$ . Conversely, if  $\text{tr}(D_s C) \geq 0$  for all positive semidefinite  $m \times m$  matrix  $C$ , then for any vector  $v$  of length  $m$  we have  $0 \leq \text{tr}(D_s v v^*) = \text{tr}(v^* D_s v) = v^* D_s v$ , hence  $D_s$  is positive semidefinite.

From the previous remark, if  $s$  is a *state* on  $M_m$ , that is, a unital positive linear functional on  $M_m$ , then  $D_s$  becomes a *density matrix*, that is, a positive semidefinite matrix of trace one. Slightly abusing this fact, we call  $D_s$  the *density matrix* associated to  $s$ , in general.

We now come back to the general case of a  $*$ -subspace  $\mathcal{S}$  in  $M_m$ . By analogy with the particular case of the operator system of full matrix algebra  $M_m$  described before, with

respect to the Hilbert-Schmidt inner product on  $M_m$ , hence on its subspace  $\mathcal{S}$ , to any linear functional  $s: \mathcal{S} \rightarrow \mathbb{C}$  one uniquely associates an  $m \times m$  matrix  $D_s \in \mathcal{S} \subseteq M_m$  such that

$$s(C) = \text{tr}(D_s^* C), \quad C \in \mathcal{S}, \tag{2.19}$$

and we continue to call  $D_s$  the *density matrix* associated to  $s$ . Clearly, this establishes a conjugate linear isomorphism between the dual space of  $\mathcal{S}$  and  $\mathcal{S}$ . In view of Theorem 2.6, we may ask whether the positivity of the linear functional  $s$  is equivalent with the positive semidefiniteness of its density matrix, as in the case of the full matrix algebra  $M_n$ . Also, if the density matrix  $D_s$  is positive semidefinite then  $s$  is a positive linear functional but, as the following remarks and examples show, the converse may or may not hold.

*Remarks 2.8*

(1) If  $\mathcal{S}$  is a  $*$ -subspace of  $M_n$  and the linear functional  $s: \mathcal{S} \rightarrow \mathbb{C}$  is Hermitian, that is,  $s(C^*) = \overline{s(C)}$  for all  $C \in \mathcal{S}$ , then its density matrix  $D$  is Hermitian. Indeed, for any  $C \in \mathcal{S}$  we have

$$s(C) = \overline{s(C^*)} = \overline{\text{tr}(D^* C^*)} = \text{tr}(CD) = \text{tr}((D^*)^* C),$$

hence,  $D^*$  is also a density matrix for  $s$ . Since the density matrix is unique, it follows that  $D = D^*$ .

(2) If  $\mathcal{S}$  is a  $C^*$ -subalgebra of  $M_m$ , not necessarily unital, then for any positive functional  $s: \mathcal{S} \rightarrow \mathbb{C}$ , its density matrix  $D$  is positive semidefinite. Indeed, in this case  $D = D_+ - D_-$  with  $D_{\pm} \in \mathcal{S}^+$  and  $D_+ D_- = 0$  hence  $0 \leq s(D_-) = \text{tr}(D D_-) = -\text{tr}(D_-^2)$  hence  $D_- = 0$  and consequently  $D \in \mathcal{S}^+$ .

*Examples 2.9*

(1) We consider the following operator system  $\mathcal{S}$  in  $M_3$

$$\mathcal{S} = \left\{ C = \begin{bmatrix} a & 0 & b \\ 0 & a & 0 \\ c & 0 & d \end{bmatrix} \mid a, b, c, d \in \mathbb{C} \right\}, \tag{2.20}$$

and note that  $\mathcal{S}^+$  consists on those matrices  $C$  as in (2.20) with  $c = \bar{b}$ ,  $a, d \geq 0$ , and  $|b|^2 \leq ad$ . Let

$$D = \begin{bmatrix} 1 & 0 & \sqrt{2} \\ 0 & 1 & 0 \\ \sqrt{2} & 0 & 1 \end{bmatrix},$$

and note that  $D \in \mathcal{S}$  is Hermitian but it is not positive semidefinite: more precisely, its eigenvalues are  $1 - \sqrt{2}$ ,  $1$ , and  $1 + \sqrt{2}$ . On the other hand, for any  $C \in \mathcal{S}^+$ , that is, with the notation as in (2.20),  $c = \bar{b}$ ,  $a, d \geq 0$ , and  $|b|^2 \leq ad$ , we have

$$\begin{aligned} \text{tr}(DC) &= a + \sqrt{2}\bar{b} + a + \sqrt{2}b + d = 2a + d + 2\sqrt{2} \text{Re } b \\ &\geq 2a + d - 2\sqrt{2}|b| \geq 2a + d - 2\sqrt{2}\sqrt{ad} = (\sqrt{2a} - \sqrt{d})^2 \geq 0, \end{aligned}$$

hence the linear functional  $\mathcal{S} \ni C \mapsto \text{tr}(DC) \in \mathbb{C}$  is positive.

(2) In  $M_2$  we consider the Pauli matrices

$$\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{2.21}$$

that makes an orthogonal basis of  $M_2$  with respect to the Hilbert-Schmidt inner product. We consider  $\mathcal{S}$  the linear span of  $\sigma_0, \sigma_1$  and  $\sigma_2$ , more precisely,

$$\mathcal{S} = \left\{ C = \begin{bmatrix} \alpha & \beta \\ \gamma & \alpha \end{bmatrix} \mid \alpha, \beta, \gamma \in \mathbb{C} \right\}. \tag{2.22}$$

Note that  $\mathcal{S}$  is an operator system but not an algebra. However, we show that, an arbitrary matrix  $D \in \mathcal{S}$  is positive semidefinite if and only if  $\text{tr}(D^*C) \geq 0$  for all  $C \in \mathcal{S}^+$ .

To this end, note that a matrix  $C$  as in (2.22) is positive semidefinite if and only if  $\gamma = \bar{\beta}$ ,  $\alpha \geq 0$ , and  $|\beta|^2 \leq \alpha^2$ . Let  $D \in \mathcal{S}$ , that is,

$$D = \begin{bmatrix} a & b \\ c & a \end{bmatrix},$$

such that  $\text{tr}(D^*C) \geq 0$  for all  $C \in \mathcal{S}^+$ . From Remark 2.8 it follows that  $D$  is Hermitian, hence  $a$  is real and  $c = \bar{b}$ , and the condition  $\text{tr}(D^*C) \geq 0$  can be equivalently written as

$$a\alpha + \text{Re}(\bar{\beta}b) \geq 0 \text{ whenever } \alpha \geq 0 \text{ and } |\beta|^2 \leq \alpha^2. \tag{2.23}$$

Letting  $\beta = 0$  implies that  $a \geq 0$ . We prove that  $|b|^2 \geq a^2$ . If  $a = 0$  then from (2.23), it follows that  $b = 0$ . If  $a > 0$  and  $|b|^2 > a^2$  then letting  $\alpha = a$  and  $\beta = -a|b|/\bar{b}$ , we obtain  $0 \leq a\alpha + \text{Re}(\bar{\beta}b) = a^2 - a|b| = a(a - |b|) < 0$ , a contradiction. Hence  $|b|^2 \geq a^2$  must hold, and we have proven that  $D$  is positive semidefinite.

### 3. Main results

#### 3.1. The general case

Let  $A_1, \dots, A_N \in M_n$  and  $B_1, \dots, B_N \in M_k$  be the given interpolation data with respect to the interpolation problem, see the Introduction. We recall the notation  $\mathbf{A} = (A_1, \dots, A_N)$ , called the *input data* and, similarly,  $\mathbf{B} = (B_1, \dots, B_N)$ , called the *output data*. We are looking for  $\varphi \in \text{CP}(M_n, M_k)$  such that the interpolation condition holds

$$\varphi(A_\nu) = B_\nu, \quad \text{for all } \nu = 1, \dots, N. \tag{3.1}$$

Since any completely positive map is Hermitian, without loss of generality we can assume that all  $A_\nu$  and all  $B_\nu$  are Hermitian, otherwise we may increase the number of the data by splitting each entry into its real and its imaginary parts, respectively. Also, without loss of generality, we can assume that  $A_1, \dots, A_N$  are linearly independent, otherwise some linearly dependence consistency conditions on  $B_1, \dots, B_N$  should be imposed. On the other hand, since the required maps  $\varphi$  should be linear, the constraint (3.1) actually determines  $\varphi$  on the linear space generated by  $A_1, \dots, A_N$

$$\mathcal{S}_{\mathbf{A}} = \text{Lin}\{A_1, \dots, A_N\}, \tag{3.2}$$

which is a  $*$ -subspace due to the fact that all  $A_\nu$  are Hermitian matrices. In conclusion, without loss of generality, we work under the following hypotheses on the data:

- (a1) All matrices  $A_1, \dots, A_N \in M_n$  and  $B_1, \dots, B_N \in M_k$  are Hermitian.
- (a2) The set of matrices  $\{A_1, \dots, A_N\}$  is linearly independent.

From now on,  $\mathcal{S}_A$  is a  $*$ -subspace of  $M_n$  for which  $A_1, \dots, A_N$  is a linear basis. Having in mind the approach of the interpolation problem through the Arveson’s Hahn-Banach Theorem and Smith-Ward linear functional,  $\mathcal{S}_A$  might be required to be linearly generated by  $\mathcal{S}_A^+$ . We will also consider special cases when, in addition to the hypotheses (a1) and (a2), the following condition might be imposed on the data:

(a3)  $\mathcal{S}_A$  is linearly generated by  $\mathcal{S}_A^+$ .

*Remark 3.1* Recalling the definition of  $\mathcal{C}_{A,B}$  as in (1.3), the set of solutions of the interpolation problem, observe that  $\mathcal{C}_{A,B}$  is convex and closed. If  $\mathcal{S}_A$  contains a positive definite matrix of rank  $n$ , in particular, if  $\mathcal{S}_A$  is an operator system, then  $\mathcal{C}_{A,B}$  is bounded as well, hence compact. Indeed, if  $\mathcal{S}_A$  is an operator system, this follows from the fact, e.g. see Proposition 3.6 in [15], that  $\|\varphi\| = \|\varphi(I_n)\|$  and, since  $I_n \in \mathcal{S}_A$ , the positive semidefinite matrix  $\varphi(I_n)$  is fixed and independent of  $\varphi \in \mathcal{C}_{A,B}$ . The general case follows now by Proposition 2.2. However, the same Proposition 2.2 shows that assuming that  $\mathcal{S}_A$  is generated by  $\mathcal{S}_A^+$  is not sufficient for the compactness of  $\mathcal{C}_{A,B}$ .

In order to approach the interpolation problem, it is natural to associate a linear map  $\varphi_{A,B}: \mathcal{S}_A \rightarrow M_k$  to the data  $A$  and  $B$  by letting

$$\varphi_{A,B}(A_v) = B_v, \quad v = 1, \dots, N, \tag{3.3}$$

and then uniquely extending it by linearity to the whole  $*$ -subspace  $\mathcal{S}_A$ . Then, having in mind the Smith-Ward linear functional (2.12), let

$$s_{A,B} \left( E_{i,j}^{(k)} \otimes A_v \right) = \left\langle B_v e_j^{(k)}, e_i^{(k)} \right\rangle_{\mathbb{C}^k} = b_{i,j,v}, \quad i, j = 1, \dots, k, \quad v = 1, \dots, N, \tag{3.4}$$

where

$$B_v = \sum_{i,j=1}^k b_{i,j,v} E_{i,j}^{(k)}, \quad v = 1, \dots, N. \tag{3.5}$$

Since  $\{E_{i,j}^{(k)} \otimes A_v \mid i, j = 1, \dots, k, v = 1, \dots, N\}$  is a basis for  $M_k \otimes \mathcal{S}_A$ , it follows that  $s_{A,B}$  admits a unique extension to a linear functional  $s_{A,B}$  on  $M_k(\mathcal{S}_A)$ . Note that, with respect to the transformations (2.12) and (2.15), the functional  $s_{A,B}$  corresponds to the map  $\varphi_{A,B}$ , and vice-versa.

To the linear functional  $s_{A,B}$  one also uniquely associates its density matrix  $D_{A,B}$  as in (2.19), more precisely,

$$s_{A,B}(C) = \text{tr}(D_{A,B}^* C), \quad C \in M_k \otimes \mathcal{S}_A, \tag{3.6}$$

that can be explicitly calculated in terms of input–output data  $A$  and  $B$ , as follows.

**PROPOSITION 3.2** *Let the data  $A_1, \dots, A_N$  and  $B_1, \dots, B_N$  satisfy the assumptions (a1) and (a2). Then, the density matrix  $D_{A,B}$  of the linear functional  $s_{A,B}$  is*

$$D_{A,B} = \sum_{v=1}^N \sum_{i,j=1}^k d_{i,j,v} E_{i,j}^{(k)} \otimes A_v, \tag{3.7}$$

where, for each pair  $i, j = 1, \dots, k$ , the numbers  $d_{i,j,1}, \dots, d_{i,j,N}$  are the unique solutions of the linear system

$$\sum_{\mu=1}^N d_{i,j,\mu} \operatorname{tr}(A_\mu A_\nu) = \bar{b}_{i,j,\nu}, \quad \nu = 1, \dots, N, \tag{3.8}$$

and the numbers  $b_{i,j,\nu}$  are defined at (3.5).

*Proof* Clearly, the density matrix  $D_{\mathbf{A},\mathbf{B}}$  can be represented in terms of the basis  $\{E_{i,j}^{(k)} \otimes A_\nu \mid i, j = 1, \dots, k, \nu = 1, \dots, N\}$  as in (3.7), so we only have to show that (3.8) holds. To this end, note that

$$D_{\mathbf{A},\mathbf{B}}^* = \sum_{i,j=1}^k \sum_{\nu=1}^N \bar{d}_{i,j,\nu} E_{j,i}^{(k)} \otimes A_\nu,$$

recalling that  $A_\nu$  are Hermitian matrices, by assumption. Then, in view of (3.4), for each  $i, j = 1, \dots, k$  and each  $\nu = 1, \dots, N$ , we have

$$\begin{aligned} b_{i,j,\nu} &= s_{\mathbf{A},\mathbf{B}} \left( E_{i,j}^{(k)} \otimes A_\nu \right) = \operatorname{tr} \left( D_{\mathbf{A},\mathbf{B}}^* \left( E_{i,j}^{(k)} \otimes A_\nu \right) \right) \\ &= \operatorname{tr} \left( \sum_{i',j'=1}^k \sum_{\mu=1}^N \bar{d}_{i',j',\mu} \left( E_{j',i'}^{(k)} E_{i,j}^{(k)} \otimes A_\mu A_\nu \right) \right) \end{aligned}$$

then, taking into account that  $E_{j',i'}^{(k)} E_{i,j}^{(k)} = \delta_{i',i} E_{j',j}^{(k)}$ , we have

$$= \sum_{\mu=1}^N \sum_{j'=1}^k \bar{d}_{i,j',\mu} \operatorname{tr} \left( E_{j',j}^{(k)} \right) \operatorname{tr}(A_\mu A_\nu)$$

and, since  $\operatorname{tr}(E_{j',j}^{(k)}) = \delta_{j',j}$ , we have

$$= \sum_{\mu=1}^N \bar{d}_{i,j,\mu} \operatorname{tr}(A_\mu A_\nu).$$

Finally, observe that the matrix  $[\operatorname{tr}(A_\mu A_\nu)]_{\mu,\nu=1}^N$  is the Gramian matrix of the linearly independent system  $A_1, \dots, A_N$  with respect to the Hilbert-Schmidt inner product, hence positive definite and, in particular, nonsingular. Therefore, the system (3.8) has unique solution.  $\square$

**THEOREM 3.3** *Let the data  $A_1, \dots, A_N \in M_n$  and  $B_1, \dots, B_N \in M_k$  be given and subject to the assumptions (a1) and (a2), let  $\varphi_{\mathbf{A},\mathbf{B}}$  be the linear map defined at (3.3), let  $s_{\mathbf{A},\mathbf{B}}$  be the linear functional defined at (3.4) and the density matrix  $D_{\mathbf{A},\mathbf{B}}$  associated to  $s_{\mathbf{A},\mathbf{B}}$  as in (2.19). Also, let  $\mathcal{S}_{\mathbf{A}}^\perp$  be the orthogonal complement space associated to  $\mathcal{S}_{\mathbf{A}}$  with respect to the Hilbert-Schmidt inner product, see (2.11).*

*The following assertions are equivalent:*

- (i) *There exists  $\varphi \in \operatorname{CP}(M_n M_k)$  such that  $\varphi(A_\nu) = B_\nu$  for all  $\nu = 1, \dots, N$ .*
- (ii) *The affine space  $D_{\mathbf{A},\mathbf{B}} + M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp$  contains at least one positive semidefinite matrix.*

*Proof*

(i)⇒(ii). Let  $\varphi \in \text{CP}(M_n, M_k)$  be such that  $\varphi(A_\nu) = B_\nu$  for all  $\nu = 1, \dots, N$ , hence  $\varphi$  extends the linear map  $\varphi_{\mathbf{A}, \mathbf{B}}$ , and let  $s_\varphi : M_k(M_n) \rightarrow \mathbb{C}$  be the Smith-Ward linear functional associated to  $\varphi$  as in (2.12). Since  $\varphi$  is completely positive, it follows that  $s_\varphi$  is positive. Further, let  $D_\varphi \in M_{kn}$  be the density matrix of  $s_\varphi$ , cf. (2.18), hence, by Remark 2.7,  $D_\varphi$  is positive semidefinite. On the other hand, since  $\varphi$  extends  $\varphi_{\mathbf{A}, \mathbf{B}}$ , it follows that  $s_\varphi$  extends  $s_{\mathbf{A}, \mathbf{B}}$ , hence  $D_\varphi = D_{\mathbf{A}, \mathbf{B}} + P$  for some  $P \in (M_k \otimes \mathcal{S}_{\mathbf{A}})^\perp = M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp$ .

(ii)⇒(i). Let  $D = D_{\mathbf{A}, \mathbf{B}} + P$  be positive semidefinite, for some  $P \in (M_k \otimes \mathcal{S}_{\mathbf{A}})^\perp = M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp$ . Then

$$\text{tr}(D^*C) = \text{tr}((D_{\mathbf{A}, \mathbf{B}}^* + P^*)C) = \text{tr}(D_{\mathbf{A}, \mathbf{B}}^*C) = s_{\mathbf{A}, \mathbf{B}}(C), \quad C \in \mathcal{S}_{\mathbf{A}},$$

hence, letting  $s : M_{kn} \rightarrow \mathbb{C}$  be the linear functional associated to the density matrix  $D$ , it follows that  $s$  is positive and extends  $s_{\mathbf{A}, \mathbf{B}}$ . Further, let  $\varphi_s : M_n \rightarrow M_k$  be the linear map associated to  $s$  as in (2.16). Then  $\varphi$  is completely positive and extends  $\varphi_{\mathbf{A}, \mathbf{B}}$ . □

**COROLLARY 3.4** *Under the assumptions and the notation of Theorem 3.3, suppose that one (hence both) of the equivalent conditions (i) and (ii) holds. Then, the formula*

$$\varphi(A) = \left[ \text{tr} \left( (D_{\mathbf{A}, \mathbf{B}} + P) \left( E_{i,j}^{(k)} \otimes A \right) \right) \right]_{i,j=1}^k, \quad A \in M_n, \tag{3.9}$$

*establishes an affine isomorphism between the closed convex sets*

$$\mathcal{C}_{\mathbf{A}, \mathbf{B}} := \{ \varphi \in \text{CP}(M_n, M_k) \mid \varphi(A_\nu) = B_\nu, \text{ for all } \nu = 1, \dots, N \}, \tag{3.10}$$

and

$$\mathcal{P}_{\mathbf{A}, \mathbf{B}} := \left\{ P \in \left( M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp \right)^h \mid P \geq -D_{\mathbf{A}, \mathbf{B}} \right\}. \tag{3.11}$$

*Proof* It is clear that both sets  $\mathcal{C}_{\mathbf{A}, \mathbf{B}}$  and  $\mathcal{P}_{\mathbf{A}, \mathbf{B}}$  are closed and convex.

The fact that the formula (3.9) establishes an affine isomorphism between these two convex sets follows, on one hand, from the affine isomorphism properties of the Smith-Ward functional and of the density matrix and, on the other hand, from the proof of Theorem 3.3. □

**Remarks 3.5** Let the assumptions and the notation of Theorem 3.3 hold.

- (1) In order for the set  $\mathcal{C}_{\mathbf{A}, \mathbf{B}}$  to be nonempty, a necessary condition is, clearly, that for any  $\nu = 1, \dots, N$ , if  $A_\nu$  is semidefinite, then  $B_\nu$  is semidefinite of the same type, that is, either positive semidefinite or negative semidefinite.
- (2) If the density matrix  $D_{\mathbf{A}, \mathbf{B}}$  is positive semidefinite, as a consequence of Corollary 3.4 the set  $\mathcal{C}_{\mathbf{A}, \mathbf{B}}$  is nonempty, more precisely, the map  $\varphi : M_n \rightarrow M_k$  defined by

$$\varphi(A) = \left[ \text{tr} \left( D_{\mathbf{A}, \mathbf{B}} \left( E_{i,j}^{(k)} \otimes A \right) \right) \right]_{i,j=1}^n, \quad A \in M_n, \tag{3.12}$$

is completely positive and  $\varphi(A_\nu) = B_\nu$  for all  $\nu = 1, \dots, N$ . We stress the fact that this sufficient condition is, in general, not necessary, see Examples 2.9.

- (3) According to Corollary 3.2 in [2], for any  $A \in M_n^+$  and  $B \in M_k^+$  there exists  $\varphi \in \text{CP}(M_n, M_k)$  such that  $\varphi(A) = B$ . This can be obtained, in our setting, by



observing that, in this case,  $D_{A,B} = B^T \otimes A$  is positive semidefinite and then apply the previous statement.

The following theorem considers the special case when the  $*$ -space  $\mathcal{S}_A$  is generated by its positive cone  $\mathcal{S}_A^+$ . This assumption, for example, becomes natural if we are looking for solutions  $\varphi$  of the interpolation problem that are unital, that is,  $\varphi(I_n) = I_k$ , or if we assume that the data  $\mathbf{A}$  and  $\mathbf{B}$  consist of quantum states. The equivalence of assertions (1) and (2), which is based on Arveson’s Hahn-Banach Theorem, has been also observed in a different setting but equivalent formulation by Jenčová, cf. Theorem 1 in [26], and by Heinosaari et al. cf. Theorem 4 and Corollary 2 in [8] (our Corollary 2.3 and Corollary 2 in [8] explains that the two cited theorems are actually equivalent).

**THEOREM 3.6** *With the assumptions and the notation as in Theorem 3.3 assume, in addition, that (a3) holds as well. The following assertions are equivalent:*

- (1) *There exists  $\varphi \in \text{CP}(M_n, M_k)$  such that  $\varphi(A_\nu) = B_\nu$  for all  $\nu = 1, \dots, N$ .*
- (2) *The linear map  $\varphi_{\mathbf{A},\mathbf{B}}$  defined at (3.3) is  $k$ -positive.*
- (3) *The linear functional  $s_{\mathbf{A},\mathbf{B}}: M_k \otimes \mathcal{S}_A \rightarrow \mathbb{C}$  defined by (3.4) is positive.*
- (4) *The affine space  $D_{\mathbf{A},\mathbf{B}} + M_k \otimes \mathcal{S}_A^+$  contains at least one positive semidefinite matrix.*

*Proof*

(1) $\Rightarrow$ (2). Let  $\varphi: M_n \rightarrow M_k$  be a completely positive map such that  $\varphi(A_\nu) = B_\nu$  for all  $\nu = 1, \dots, N$ . Then  $\varphi|_{\mathcal{S}_A}: \mathcal{S}_A \rightarrow M_k$  is completely positive, in the sense specified at the beginning of Section 2.3, that is,  $\varphi_{\mathbf{A},\mathbf{B}} = \varphi|_{\mathcal{S}_A}$  is completely positive, in particular  $k$ -positive.

(2) $\Rightarrow$ (3). Assume that  $\varphi_{\mathbf{A},\mathbf{B}}$  is  $k$ -positive. With notation as in (2.13), a moment of thought shows that, for each  $i, j = 1, \dots, N$  and each  $\nu = 1, \dots, N$ , we have

$$\left\langle (I_k \otimes \varphi_{\mathbf{A},\mathbf{B}}) \left( E_{i,j}^{(k)} \otimes A_\nu \right) e^{(k)}, e^{(k)} \right\rangle_{\mathbb{C}^{k^2}} = \varphi_{\mathbf{A},\mathbf{B}}(A_\nu) = B_\nu = s_{\mathbf{A},\mathbf{B}} \left( E_{i,j}^{(k)} \otimes A_\nu \right),$$

hence

$$\left\langle (I_k \otimes \varphi_{\mathbf{A},\mathbf{B}}) (C) e^{(k)}, e^{(k)} \right\rangle_{\mathbb{C}^{k^2}} = s_{\mathbf{A},\mathbf{B}}(C), \quad C \in M_k \otimes \mathcal{S}_A, \quad (3.13)$$

and, consequently,  $s_{\mathbf{A},\mathbf{B}}$  maps any positive semidefinite matrix from  $M_k \otimes \mathcal{S}_A$  to a nonnegative number.

(3) $\Rightarrow$ (1). Assume that the linear functional  $s_{\mathbf{A},\mathbf{B}}: M_k \otimes \mathcal{S}_A \rightarrow \mathbb{C}$  defined by (3.4) is positive, in the sense that it maps any positive element in  $M_k \otimes \mathcal{S}_A = M_k(\mathcal{S}_A)$  into  $\mathbb{R}_+$ . By Arveson’s Hahn-Banach Theorem, [16] see the implication (c) $\Rightarrow$ (d) in Theorem 2.6 and the argument provided there, there exists a completely positive map  $\tilde{\varphi}: M_k \rightarrow M_n$  extending  $\varphi_{\mathbf{A},\mathbf{B}}$ , hence  $\tilde{\varphi}$  satisfies the same interpolation constraints as  $\varphi_{\mathbf{A},\mathbf{B}}$ .

(1) $\Leftrightarrow$ (4). Proven in Theorem 3.3. □

**Remark 3.7** Under the assumptions and notation as in Theorem 3.6, if  $\mathcal{S}_A$  contains a positive definite matrix, then the set  $\mathcal{C}_{\mathbf{A},\mathbf{B}}$  is convex and compact, see Remark 3.1. Then the set  $\mathcal{P}_{\mathbf{A},\mathbf{B}}$ , see Corollary 3.4, is convex and compact as well.

**COROLLARY 3.8** *If the  $*$ -subspace  $\mathcal{S}_A$  is an algebra, then the set  $\mathcal{C}_{A,B}$  is nonempty if and only if  $D_{A,B}$  is positive semidefinite, more precisely, in this case (3.12) provides a solution  $\varphi \in \mathcal{C}_{A,B}$  of the interpolation problem.*

*Proof* This is a consequence of Theorem 3.6, the second statement of Remark 2.8, and the second statement of Remark 3.5. □

Example 2.9.(2) shows that the statement in the previous corollary may be true without the assumption that the  $*$ -space  $\mathcal{S}_A$  is an algebra.

**Remark 3.9** *Trace Preserving.* Recall that a linear map  $\varphi: M_n \rightarrow M_k$  is *trace preserving* if  $\text{tr}(\varphi(A)) = \text{tr}(A)$  for all  $A \in M_n$ . With the notation as in Theorem 3.3, let

$$\mathcal{Q}_{A,B} := \{\varphi \in \mathcal{C}_{A,B} \mid \varphi \text{ is trace preserving}\}, \tag{3.14}$$

and we want to determine, with respect to the affine isomorphism established in Corollary 3.4, how the corresponding parameterizing subset  $\mathcal{P}_{A,B}$  can be singled out and, implicitly, to get a characterization of the solvability of the interpolation problem for quantum channels. So let  $P = [p_{(i,l),(j,m)}]$  be an arbitrary matrix in  $\mathcal{P}_{A,B}$ , where  $(i, l) = (i - 1)n + l$  and  $(j, m) = (j - 1)n + m$ , for  $i, j = 1, \dots, k$  and  $l, m = 1, \dots, n$ , equivalently, in tensor notation,

$$P = \sum_{i,j=1}^k \sum_{l,m=1}^n p_{(i,l),(j,m)} E_{i,j}^{(k)} \otimes E_{l,m}^{(n)}.$$

In view of (3.9), a map  $\varphi \in \mathcal{C}_{A,B}$  is trace invariant if and only if

$$\text{tr} \left( \varphi \left( E_{l,m}^{(n)} \right) \right) = \text{tr} \left( E_{l,m}^{(n)} \right) = \delta_{l,m}, \quad l, m = 1, \dots, n, \tag{3.15}$$

which, taking into account of Proposition 3.2, is equivalent with the conjunction of the following affine constraints

$$\sum_{i=1}^k p_{(i,m),(i,l)} = \delta_{l,m} - \sum_{v=1}^N a_{m,l,v} \left( \sum_{i=1}^k d_{i,i,v} \right), \quad l, m = 1, \dots, n. \tag{3.16}$$

**Remark 3.10** Assume that  $\mathcal{S}_A$  is an operator system. By Theorem 3.3, if the interpolation problem has a solution then there exists a positive semidefinite matrix  $\tilde{D}$  in  $D_{A,B} + M_k \otimes \mathcal{S}_A^\perp$  hence, by Lemma 2.5 we have  $0 \leq \text{tr}(\tilde{D}) = \text{tr}(D_{A,B})$ . Therefore, under these assumptions, a necessary condition of solvability of the interpolation problem is  $\text{tr}(D_{A,B}) \geq 0$ .

**3.2. Orthonormalization of the input data**

Theorem 3.3 gives the necessary and sufficient condition of solvability of the interpolation problem in terms of the density matrix  $D_{A,B}$  but, in order to precisely get it one might solve the system of linear equations (3.8), with the Gramian matrix  $[\text{tr}(A_\mu^* A_\nu)]_{\mu,\nu}$  as the principal matrix of the system. If the matrices  $A_1, \dots, A_N$  are mutually orthogonal with respect to the Hilbert-Schmidt inner product, this Gramian matrix is just the identity matrix  $I_N$ . Observe that, if this is not the case, applying the Gram-Schmidt orthonormalization algorithm to the linearly independent input Hermitian matrices  $A_1, \dots, A_N$ , we obtain an orthonormal

system of matrices that preserves all assumptions (a1)–(a3), due to the fact that the trace of a product of two Hermitian matrices is always real. More precisely, if  $A'_1, \dots, A'_N$  is the Gram-Schmidt orthogonalization of the sequence of linearly independent Hermitian matrices  $A_1, \dots, A_N$  then

$$A'_1 = \frac{1}{\sqrt{\text{tr}(A_1^2)}} A_1,$$

$$U_{v+1} = A_{v+1} - \sum_{\mu=1}^v \text{tr}(A'_\mu A_\mu) A_\mu, \quad A'_{v+1} = \frac{1}{\sqrt{\text{tr}(U_{v+1}^2)}} U_{v+1}, \quad v = 1, \dots, N - 1.$$

Then, we can change, accordingly, the sequence  $B_1, \dots, B_N$  to  $B'_1, \dots, B'_N$

$$B'_1 = \frac{1}{\sqrt{\text{tr}(A_1^2)}} B_1, \quad B'_{v+1} = \frac{1}{\sqrt{\text{tr}(U_{v+1}^2)}} \left( B_{v+1} - \sum_{\mu=1}^v \text{tr}(A'_\mu A_\mu) B_\mu \right), \quad v = 1, \dots, N - 1,$$

and observe that a linear map  $\varphi: M_n \rightarrow M_k$  satisfies the constraints  $\varphi(A_v) = B_v$ ,  $v = 1, \dots, N$ , if and only if  $\varphi(A'_v) = B'_v$ ,  $v = 1, \dots, N$ . Therefore, without loss of generality, we can replace the assumption (a2) with the assumption

(a2') *The set of matrices  $\{A_1, \dots, A_N\}$  is orthonormal with respect to the Hilbert-Schmidt inner product, that is,  $\text{tr}(A_\mu A_\nu) = \delta_{\mu,\nu}$  for all  $\mu, \nu = 1, \dots, N$ .*

LEMMA 3.11 *Under the assumptions (a1) and (a2'), the density matrix  $D_{\mathbf{A},\mathbf{B}}$  of the linear functional  $s_{\mathbf{A},\mathbf{B}}$  defined at (3.4) is*

$$D_{\mathbf{A},\mathbf{B}} = \sum_{v=1}^N B_v^T \otimes A_v. \tag{3.17}$$

*Proof* Under the assumption (a2'), the Gramian matrix of  $A_1, \dots, A_N$  is the identity matrix  $I_N$  hence the system of linear equations (3.8) is simply solvable as  $d_{i,j,v} = \bar{b}_{i,j,v} = b_{j,i,v}$  for all  $i, j = 1, \dots, k$  and all  $v = 1, \dots, N$ , where we have taken into account that  $B_v$  are all Hermitian matrices. By (3.7) we have

$$D_{\mathbf{A},\mathbf{B}} = \sum_{v=1}^N \sum_{i,j=1}^k b_{j,i,v} E_{i,j}^{(k)} \otimes A_v = \sum_{v=1}^N B_v^T \otimes A_v.$$

□

Note that under the assumptions (a1) and (a2') we can always find an orthonormal basis  $A_1, \dots, A_N, A_{N+1}, \dots, A_{n^2}$  of  $M_n$ , with respect to the Hilbert-Schmidt inner product, whose first  $N$  elements are exactly the elements of the input data  $\mathbf{A}$  and such that all its matrices are Hermitian. Indeed, this basically follows from the fact that  $\mathcal{S}_{\mathbf{A}}^\perp$  is a  $*$ -space, and the remark we made before on the Gram-Schmidt orthonormalization of a sequence of linearly independent Hermitian matrices.

THEOREM 3.12 *Assume that the data  $A_1, \dots, A_N$  and  $B_1, \dots, B_N$  satisfy the assumptions (a1) and (a2'). Let  $A_{N+1}, \dots, A_{n^2}$  be a sequence of Hermitian matrices in  $M_n$  such that*

$A_1, \dots, A_{n^2}$  is an orthonormal basis of  $M_n$  with respect to the Hilbert-Schmidt inner product. The following assertions are equivalent:

- (1) There exists  $\varphi \in \text{CP}(M_n, M_k)$  such that  $\varphi(A_\nu) = B_\nu$  for all  $\nu = 1, \dots, N$ .
- (2) There exist numbers  $p_{i,j,\nu}$ ,  $i, j = 1, \dots, k$  and  $\nu = N + 1, \dots, n^2$ , such that  $p_{j,i,\nu} = \overline{p_{i,j,\nu}}$  and

$$\sum_{\nu=1}^N B_\nu^T \otimes A_\nu + \sum_{i,j=1}^k \sum_{\nu=N+1}^{n^2} p_{i,j,\nu} E_{i,j}^{(k)} \otimes A_\nu \geq 0. \tag{3.18}$$

*Proof* We use Theorem 3.3, by means of Lemmas 3.11 and 2.5, taking into account that in order to get a positive semidefinite matrix in the affine space  $D_{\mathbf{A},\mathbf{B}} + M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp$  we actually look for a Hermitian element  $P \in M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp$ , more precisely

$$P = \sum_{i,j=1}^k \sum_{\nu=N+1}^{n^2} p_{i,j,\nu} E_{i,j}^{(k)} \otimes A_\nu,$$

such that  $D_{\mathbf{A},\mathbf{B}} + P \geq 0$ . □

*Remarks 3.13* Assume that the data  $A_1, \dots, A_N$  and  $B_1, \dots, B_N$  satisfy the assumptions (a1) and (a2').

- (i) If the set  $\mathcal{C}_{\mathbf{A},\mathbf{B}}$  is nonempty and  $\mathcal{S}_{\mathbf{A}}$  is an operator system, then, as a consequence of Lemma 3.11 and Remark 3.5,  $\sum_{\nu=1}^N \text{tr}(B_\nu) \text{tr}(A_\nu) \geq 0$ .
- (ii) On the other hand, from Lemma 3.11 and Remark 3.5.(2), if

$$\sum_{\nu=1}^N B_\nu^T \otimes A_\nu \geq 0, \tag{3.19}$$

then the linear map  $\varphi: M_n \rightarrow M_k$  defined by

$$\varphi(C) = \left[ \sum_{\nu=1}^N b_{i,j,\nu} \text{tr}(A_\nu C) \right]_{i,j=1}^k, \quad C \in M_n, \tag{3.20}$$

where  $b_{i,j,\nu}$  are the entries of the matrix  $B_\nu$ , see (3.5), is completely positive and satisfies the interpolation constraints  $\varphi(A_\nu) = B_\nu$  for all  $\nu = 1, \dots, N$ .

### 3.3. A single interpolation pair

For fixed  $n, k \in \mathbb{N}$ , consider completely positive maps  $\varphi: M_n \rightarrow M_k$  in the minimal Kraus representation, that is,  $\varphi(A) = V^*AV$ , for some  $V \in M_{k,n}$  and all  $A \in M_n$ . This corresponds to the case when the rank of the Choi matrix  $\Phi$  of  $\varphi$  is 1. For given Hermitian matrices  $A \in M_n$  and  $B \in M_k$ , we are interested to determine under which conditions on  $A$  and  $B$  there exists a completely positive maps  $\varphi$  in the minimal Kraus representation such that  $\varphi(A) = B$ .

If  $A$  is a Hermitian  $n \times n$  matrix, we consider the decomposition  $A = |A|^{1/2}S_A|A|^{1/2}$ , where  $|A| = (A^*A)^{1/2}$  is its absolute value, while  $S_A = \text{sgn}(A)$  is a Hermitian partial isometry, where  $\text{sgn}$  is the usual sign function:  $\text{sgn}(t) = 1$  for  $t > 0$ ,  $\text{sgn}(t) = -1$  for  $t < 0$ , and  $\text{sgn}(0) = 0$ , and we use functional calculus for the Hermitian matrix  $A$ . Note that, with this notation,  $A = S_A|A|$  is the polar decomposition of  $A$ . Let  $\mathcal{H}_A = \mathbb{C}^n \ominus \ker(A)$  and, further, consider the decomposition  $\mathcal{H}_A = \mathcal{H}_A^+ \oplus \mathcal{H}_A^-$ , where  $\mathcal{H}_A^\pm$  is the spectral subspace of  $S_A$  (and of  $A$ , as well) corresponding, respectively, to the eigenvalue  $\pm 1$ . Then, with respect to the decomposition

$$\mathbb{C}^n = \mathcal{H}_A^+ \oplus \mathcal{H}_A^- \oplus \ker(A), \tag{3.21}$$

we have

$$A = \begin{bmatrix} A_+ & 0 & 0 \\ 0 & -A_- & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad S_A = \begin{bmatrix} I_A^+ & 0 & 0 \\ 0 & -I_A^- & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{3.22}$$

where  $A_\pm$  act in  $\mathcal{H}_A^\pm$ , respectively, are positive operators, and  $I_A^\pm$  are the identity operators in  $\mathcal{H}_A^\pm$ , respectively.

With this notation, we consider the *signatures*  $\kappa_\pm(A) = \dim(\mathcal{H}_A^\pm) = \text{rank}(A_\pm)$  and  $\kappa_0(A) = \dim(\ker(A))$ . The triple  $(\kappa_-(A), \kappa_0(A), \kappa_+(A))$  is called the *inertia* of  $A$ . Note that  $\kappa_\pm(A)$  is the number of positive/negative eigenvalues of the matrix  $A$ , counted with their multiplicities, as well as the *number of negative/positive squares* of the quadratic form  $\mathbb{C}^n \ni x \mapsto \langle Ax, x \rangle$ . In this respect, the space  $\mathbb{C}^n$  has natural structure of *indefinite inner product* with respect to

$$[x, y]_A = \langle Ax, y \rangle, \quad x, y \in \mathbb{C}^n. \tag{3.23}$$

Then,  $\kappa_\pm(A)$  coincides with the dimension of any  $A$ -maximal positive/negative subspace: here, a subspace  $\mathcal{L} \in \mathbb{C}^n$  is called *positive* if  $[x, x]_A > 0$  for all nonnull  $x \in \mathcal{L}$ .

**LEMMA 3.14** *Let  $A \in M_n$  and  $B \in M_k$  be two Hermitian matrices. Then, there exists a completely positive map  $\varphi$  with minimal Kraus (Choi) rank equal to 1 and such that  $\varphi(A) = B$  if and only if  $\kappa_\pm(B) \leq \kappa_\pm(A)$ .*

*Proof* Assume that  $B = V^*AV$  for some  $V \in M_{k,n}$  and note that for all nonnull  $x \in \mathcal{H}_B^+$  we have

$$0 < [x, x]_B = \langle Bx, x \rangle = \langle V^*AVx, x \rangle = \langle AVx, Vx \rangle = [Vx, Vx]_A,$$

hence, the subspace  $V\mathcal{H}_B^+$  is  $A$ -positive, and this implies that  $\kappa_+(B) \leq \kappa_+(A)$ . Similarly, we have  $\kappa_-(B) \leq \kappa_-(A)$ .

Conversely, let us assume that  $\kappa_\pm(B) \leq \kappa_\pm(A)$ , that is,  $\dim(\mathcal{H}_B^\pm) \leq \dim(\mathcal{H}_A^\pm)$ , and hence there exists isometric operators  $J_\pm: \mathcal{H}_B^\pm \rightarrow \mathcal{H}_A^\pm$ . In addition to the decomposition (3.21) of  $\mathbb{C}^n$  with respect to  $A$ , we consider the like decomposition of  $\mathbb{C}^k$  with respect to  $B$

$$\mathbb{C}^k = \mathcal{H}_B^+ \oplus \mathcal{H}_B^- \oplus \ker(B), \tag{3.24}$$

and with respect to it, the block-matrix representation of  $B$  similar to (3.22). Then, with respect to (3.21) and (3.24) define  $V \in M_{k,n}$  by

$$V = \begin{bmatrix} B_+^{1/2} J_+ A_+^{-1/2} & 0 & 0 \\ 0 & B_-^{1/2} J_- A_-^{-1/2} & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{3.25}$$

and then, a simple calculation shows that  $V^*AV = B$ . □

**THEOREM 3.15** *Let  $A \in M_n$  and  $B \in M_k$  be two Hermitian matrices. Then the following assertions are equivalent:*

- (i) *There exists a completely positive map  $\varphi: M_n \rightarrow M_k$  such that  $\varphi(A) = B$ .*
- (ii) *If  $A$  is semidefinite, then  $B$  is semidefinite of the same type (positive/negative).*
- (iii) *There exists  $m \in \mathbb{N}$  such that*

$$\kappa_{\pm}(B) \leq m \kappa_{\pm}(A). \tag{3.26}$$

*In addition, the minimal Kraus (Choi) rank  $r$  of a completely positive map  $\varphi: M_n \rightarrow M_k$  such that  $\varphi(A) = B$  is*

$$r = \min\{m \in \mathbb{N} \mid \kappa_{\pm}(B) \leq m \kappa_{\pm}(A)\}. \tag{3.27}$$

*Proof* It takes only a moment of thought to see that the assertions (ii) and (iii) are equivalent. Therefore, it remains to prove that the assertions (i) and (iii) are equivalent. Assuming that there exists  $m \in \mathbb{N}$  satisfying (3.26), let  $r \in \mathbb{N}$  be defined as in (3.27). Then there exist Hermitian matrices  $B_1, B_2, \dots, B_r \in M_k$  such that  $B = B_1 + B_2 + \dots + B_r$   $\kappa_{\pm}(B_j) \leq \kappa_{\pm}(A)$  for all  $j = 1, \dots, r$ . By Lemma 3.14 there exist  $V_1, V_2, \dots, V_r \in M_{k,n}$  such that  $V_j^*AV_j = B_j$  for all  $j = 1, \dots, r$ . Then, letting  $\varphi = \sum_{j=1}^r V_j^* \cdot V_j: M_n \rightarrow M_k$  we obtain a completely positive map such that  $\varphi(A) = B$ .

On the other hand, if  $V_1, V_2, \dots, V_m \in M_{k,n}$  are such that  $\sum_{j=1}^m V_j^*AV_j = B$  then for each  $j = 1, \dots, m$  we have  $\kappa_{\pm}(V_j^*AV_j) \leq \kappa_{\pm}(A)$ , hence  $\kappa_{\pm}(B) \leq \sum_{j=1}^m \kappa_{\pm}(V_j^*AV_j) \leq m\kappa_{\pm}(A)$ , hence  $r \leq m$ . □

Note that Theorem 3.15 provides one more (different) argument for Corollary 3.2 in [2], and different from the argument given in Remark 3.5.(3) as well.

### 4. Further results on density matrices

In this section, we consider two questions related to density matrices, first, the relation of density matrices with Choi matrices and, second, the relation between the positivity of linear functionals on  $*$ -subspaces generated by unit matrices with the positivity of their density matrices.

#### 4.1. Density matrices vs. Choi matrices

Since the correspondence between linear maps  $\varphi: M_n \rightarrow M_k$  and Choi matrices  $\Phi_{\varphi} \in M_{kn}$  is a linear isomorphism and, via the Smith-Ward linear functional  $s_{\varphi}$ , the correspondence

between  $\varphi$  and the density matrix  $D_{s_\varphi}$  is a conjugate linear isomorphism, it is natural to ask for an explicit relation between the Choi matrix  $\Phi_\varphi$  and  $D_{s_\varphi}$ . In order to do this, we first recall the definition of the *canonical shuffle* operators. Briefly, this comes from the two canonical identifications of  $\mathbb{C}^n \otimes \mathbb{C}^k$  with  $\mathbb{C}^{kn}$ , more precisely, for each  $l \in \{1, \dots, n\}$  and each  $i \in \{1, \dots, k\}$ , we let

$$U e_{(i-1)n+l}^{(kn)} = e_{(l-1)k+i}^{(kn)}. \tag{4.1}$$

It is clear that  $U$  is a unitary operator  $\mathbb{C}^{kn} \rightarrow \mathbb{C}^{kn}$ , hence an orthogonal  $kn \times kn$  matrix. Also, for a matrix  $X$ , out of the adjoint matrix  $X^*$ , we consider its transpose  $X^T$  as well as its entrywise complex conjugate  $\bar{X}$ .

**PROPOSITION 4.1** *For any linear map  $\varphi: M_n \rightarrow M_k$  and letting  $\Phi$  denote its Choi matrix, cf. (2.1), the density matrix  $D$  associated to the Smith-Ward linear functional  $s_\varphi$ , cf. (2.18) and (2.12), is*

$$D = U^* \bar{\Phi} U, \tag{4.2}$$

where  $U$  is the canonical shuffle unitary operator defined at (4.1).

*Proof* We first note that  $\{E_{i,j}^{(k)} \otimes E_{l,m}^{(n)} \mid i, j = 1, \dots, k, l, m = 1, \dots, n\}$  is an orthonormal basis of  $M_k \otimes M_n$  with respect to the Hilbert-Schmidt inner product, and that, with respect to the canonical identification of  $M_k \otimes M_n \simeq M_k(M_n)$ , that is, when viewed as block  $k \times k$  matrices with each entry an  $n \times n$  matrix, with  $M_{kn}$ , we have

$$E_{i,j}^{(k)} \otimes E_{l,m}^{(n)} = E_{(i-1)n+l, (j-1)n+m}^{(kn)}, \quad i, j = 1, \dots, k, l, m = 1, \dots, n.$$

Fix  $i, j \in \{1, \dots, k\}$  and  $l, m \in \{1, \dots, n\}$ . Then,

$$\begin{aligned} s_\varphi \left( E_{i,j}^{(k)} \otimes E_{l,m}^{(n)} \right) &= s_\varphi \left( E_{(i-1)n+l, (j-1)n+m}^{(kn)} \right) \\ &= \text{tr} \left( D^* E_{(i-1)n+l, (j-1)n+m}^{(kn)} \right) = \bar{d}_{(i-1)n+l, (j-1)n+m}, \end{aligned} \tag{4.3}$$

where  $D = [d_{r,s}]_{r,s=1}^{kn}$  is the matrix representation of  $D$ , more precisely,

$$D = \sum_{r,s=1}^{kn} d_{r,s} E_{r,s}^{(kn)}.$$

On the other hand, from (2.4) we have

$$s_\varphi \left( E_{i,j}^{(k)} \otimes E_{l,m}^{(n)} \right) = \langle \varphi \left( E_{l,m}^{(n)} \right) e_j^{(k)}, e_i^{(k)} \rangle_{\mathbb{C}^k} = \varphi_{(l-1)k+i, (m-1)k+j}. \tag{4.4}$$

Therefore, in view of (4.3) and (4.4) we have

$$\bar{d}_{(i-1)n+l, (j-1)n+m} = s_\varphi \left( E_{i,j}^{(k)} \otimes E_{l,m}^{(n)} \right) = \varphi_{(l-1)k+i, (m-1)k+j},$$

hence, taking into account of the definition of the canonical shuffle operator  $U$  as in (4.1), the equality in (4.2) follows.  $\square$

The concept of density matrices associated to linear functionals on  $*$ -subspaces opens the possibility of generalizing the concept of a Choi matrix for linear maps with domains  $*$ -subspaces. Note that the definition of the Choi matrix, see (2.1), involves essentially the



matrix units which, generally, are not available in operator systems. However, in view of Proposition 4.1 we can proceed as follows. First consider the Smith-Ward functional  $s_\varphi$  defined as in (2.12), then consider the density matrix  $D_\varphi$  associated to  $s_\varphi$  as in (2.19), and finally define  $\Phi_\varphi$  by

$$\Phi_\varphi = U \overline{D_\varphi} U^*, \tag{4.5}$$

where the bar denotes the entrywise complex conjugation and  $U$  denotes the canonical shuffle unitary operator as in (4.1). Clearly  $\Phi_\varphi$  is an  $kn \times kn$  matrix and, in case  $\varphi \in \text{CP}(\mathcal{S}, M_k)$ , the Choi matrix  $C_\varphi$  defined as in (4.5) is Hermitian but, at this level of generality, depending on the  $*$ -subspace  $\mathcal{S}$ , its positive definiteness is not guaranteed. However, if the Choi matrix  $\Phi_\varphi$  is positive semidefinite, then  $\varphi \in \text{CP}(\mathcal{S}, M_k)$ .

**4.2. Operator systems generated by matrix units**

For a fixed natural number  $m$  let  $\mathcal{S}$  be an operator system in  $M_m$ . We are interested by the special case when  $\mathcal{S}$  is linearly generated by a subset of matrix units in  $M_m$ , that is, there exists a subset  $S \subseteq \{1, \dots, m\}^2$  such that  $\mathcal{S} = \text{Lin}\{E_s^{(m)} \mid s \in S\}$ .

*Remarks 4.2* In the following, we use the interpretation of subsets  $S \subseteq \{1, \dots, m\}^2$  as relations on the set  $\{1, \dots, m\}$ . Let  $S$  be a relation on  $\{1, \dots, m\}$  and let  $\mathcal{S} = \text{Lin}\{E_s^{(m)} \mid s \in S\}$  be the linear subspace in  $M_m$  generated by the matrix units indexed in  $S$ .

- (1) The linear space  $\mathcal{S}$  is an operator system in  $M_m$  if and only if  $S$  is reflexive and symmetric.
- (2) The linear space  $\mathcal{S}$  is a  $*$ -subspace generated by  $\mathcal{S}^+$  if and only if, modulo a permutation of indices,  $\mathcal{S} = \mathcal{S}' \oplus 0$ , where  $\mathcal{S}'$  is an operator system in  $M_{m'}$  for some  $0 \leq m' \leq m$ . To see this, we observe that, if  $i \neq j$  are such that  $(i, j) \in S$ , then necessarily  $(i, i) \in S$  and  $(j, j) \in S$  since, otherwise,  $\mathcal{S}$  may contain matrices of type

$$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \oplus 0, \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \oplus 0,$$

that are Hermitian but cannot be written as linear combinations of matrices in  $\mathcal{S}^+$ .

- (3) The linear space  $\mathcal{S}$  is a unital  $*$ -subalgebra of  $M_m$  if and only if  $S$  is an equivalence relation.

**THEOREM 4.3** *Let  $\mathcal{S}$  be a  $*$ -subspace in  $M_m$  that is linearly generated by matrix units and also linearly generated by  $\mathcal{S}^+$ . The following assertions are equivalent:*

- (a) Any positive linear functional  $s : \mathcal{S} \rightarrow \mathbb{C}$  has a positive semidefinite density matrix.
- (b)  $\mathcal{S}$  is an algebra.

*Proof* (a) $\Rightarrow$ (b). We divide the proof in four steps.

*Step 1* We first observe that, without loss of generality, we can assume that  $\mathcal{S}$  is an operator system. Indeed, since  $\mathcal{S}$  is linearly generated by  $\mathcal{S}^+$ , by Remark 4.2.(2), modulo a permutation of indices,  $\mathcal{S} = \mathcal{S}' \oplus 0$  where  $\mathcal{S}'$  is an operator system in  $M_{m'}$  for some  $0 \leq m' \leq m$ .

*Step 2* First observe that for  $m = 1$  or  $m = 2$  any operator system  $\mathcal{S} \subseteq M_m$  generated by a set of matrix units is an algebra hence, in view of Remark 2.8.(2), there is nothing to prove.

*Step 3* We consider  $m = 3$  so let  $\mathcal{S}$  be an operator system in  $M_3$  and let  $S \subseteq \{1, 2, 3\}^2$  be the associated reflexive and symmetric relation as in Remark 4.2. Then  $S$  necessarily contains all the diagonal  $S_d = \{(1, 1), (2, 2), (3, 3)\}$ . On the other hand, due to the symmetry condition on  $S$ , it may contain only 3, 5, 7 or 9 elements. If  $S$  contains either 3, 5 or 9 elements it is easy to see that  $\mathcal{S}$  is an algebra. Consequently, we are left only with the investigation of the case when  $S$  has exactly 7 elements, and these are the cases when  $S = S_d \cup \{(1, 2), (2, 1), (1, 3), (3, 1)\}$ ,  $S = S_d \cup \{(1, 2), (2, 1), (3, 2), (2, 3)\}$ ,  $S = S_d \cup \{(2, 3), (3, 2), (1, 3), (3, 1)\}$ . Note that these three cases correspond to a circular permutation of one of them and hence the proof for any one of these would be sufficient.

Let  $S = \{(1, 1), (2, 2), (3, 3), (1, 2), (2, 1), (1, 3), (3, 1)\}$ . In the following, we prove that the corresponding operator system  $\mathcal{S} = \text{Lin } S$ , that is not an algebra, has at least one (actually we prove that there are infinitely many) positive linear functional whose density matrix is not positive semidefinite. To see this, first note that

$$\mathcal{S} = \left\{ C = \begin{bmatrix} a & b & c \\ f & d & 0 \\ g & 0 & e \end{bmatrix} \mid a, b, c, d, e, f, g \in \mathbb{C} \right\}, \tag{4.6}$$

and that  $\mathcal{S}^+$  is the collection of all matrices  $C$  as in (4.6) subject to the following conditions

$$a \geq 0, d \geq 0, e \geq 0, f = \bar{b}, g = \bar{c}, |b|^2 \leq ad, |c|^2 \leq ae, |b|^2e + |c|^2d \leq ade. \tag{4.7}$$

For each  $1/\sqrt{2} < \rho \leq 1$  consider the Hermitian matrix

$$D_\rho = \begin{bmatrix} 1 & \rho & \rho \\ \rho & 1 & 0 \\ \rho & 0 & 1 \end{bmatrix}. \tag{4.8}$$

It is easy to see that  $D_\rho$  is indefinite for each  $1/\sqrt{2} < \rho \leq 1$ .

We prove that the corresponding functional  $s_\rho = \text{tr}(D_\rho \cdot)$  is positive for each  $1/\sqrt{2} < \rho \leq 1$ . To see this, let  $C \in \mathcal{S}^+$  be arbitrary, that is, with the notation as in (4.6), the conditions (4.7) must hold. Then

$$\begin{aligned} s_\rho(C) &= \text{tr}(D_\rho C) = a + d + e + 2\rho \text{Re}(b + c) \\ &\geq a + d + e - 2\rho(|b| + |c|) \end{aligned}$$

and then, taking into account that  $|b| + |c|$  has its maximal value  $\sqrt{a(e+d)}$  when the constraints (4.7) hold and that  $\rho \leq 1$ ,

$$\geq a + d + e - 2\sqrt{a(e+d)} = (\sqrt{a} - \sqrt{e+d})^2 \geq 0.$$

*Step 4* Assume now that  $m > 3$  and assume that  $\mathcal{S}$  is an operator system in  $M_m$  that is not an algebra. By Remark 4.2.(2), there exist distinct  $i, j, l \in \{1, \dots, m\}$  such that  $(i, j), (j, l) \in S$  but  $(i, l) \notin S$ . Modulo a reindexing, without loss of generality we can assume that  $i = 2, j = 1$ , and  $l = 3$ . For each  $1/\sqrt{2} < \rho \leq 1$  we consider the matrix  $D_\rho$  as in (4.8) and let  $\tilde{D}_\rho = D_\rho \oplus 0 \in M_m$ . From what has been proven in Step 3, it follows

that the functional  $s_\rho = \text{tr}(\tilde{D}_\rho \cdot)$  on  $M_m$  is positive but its density matrix  $\tilde{D}_\rho$  is not positive semidefinite.

(b) $\Rightarrow$ (a). This is a consequence of Remark 2.8.(2).  $\square$

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