AN INTERPOLATION PROBLEM FOR COMPLETELY POSITIVE MAPS ON MATRIX ALGEBRAS: SOLVABILITY AND PARAMETRISATION

CĂLIN AMBROZIE AND AURELIAN GHEONDEA

ABSTRACT. We present certain existence criteria and parameterisations 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. We perform a careful investigation on the intricate relation between the positivity of the density matrix and the positivity of the corresponding linear functional. A necessary and sufficient condition for the existence of solutions and a parametrisation 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.

1. INTRODUCTION

The most general mathematical model of state changes in quantum mechanics, including the evolution of an open system or the state change due to a measurement, is provided by the concept of "quantum operation", that is, a linear, completely positive, trace preserving map, cf. K. Kraus [14] and [15]. 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 $\varphi \colon M_n \to M_k$ is *completely positive* if, for all $m \in \mathbb{N}$, the linear map $I_m \otimes \varphi \colon M_m \otimes M_n \to M_m \otimes M_k$ 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 $\mathrm{CP}(M_n, M_k)$ we denote the cone of all completely positive maps $\varphi \colon M_n \to M_k$. An equivalent notion, cf. W.F. Stinespring [21], is that of *positive semidefinite* map φ, 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

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

A *quantum channel* 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. Thus, P.M. Alberti and A. Uhlmann [1] 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 A. Chefles, R. Jozsa, A. Winter [4] and the bibliography cited there.

In this article we consider the following

Interpolation Problem.   *Given matrices $A_\nu \in M_n$ and $B_\nu \in M_k$ for $\nu = 1, \ldots, N$, determine $\varphi \in \mathrm{CP}(M_n, M_k)$ subject to the conditions*

$$(1.2) \qquad\qquad \varphi(A_\nu) = B_\nu, \ \text{for all } \nu = 1, \ldots, N.$$

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 φ, secondly, one should find an explicit parametrisation 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 operations. In this general formulation, these problems have been considered by C.-K. Li and Y.-T. Poon in [16], where solutions have been obtained in case when the given states (more generally, Hermitian matrices) commute. More general criteria for existence of solutions have been considered by Z. Huang, C.-K. Li, E. Poon, and N.-S. Sze in [10], while T. Heinosaari, M.A. Jivulescu, D. Reeb, and M.M. Wolf 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 Y. Nesterov and A. Nemirovsky [17] and L. Vanderberghe and S. Boyd [22].

The purpose of this article is to approach, from a general perspective, existence criteria and parametrisations of solutions of the Interpolation Problem. The solvability of the Interpolation Problem is characterised in Theorem 3.4 from which an explicit parametrisation of the set of all solutions in terms of a closed and convex set of an affine space follows.

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

$$(1.3) \qquad \mathcal{C}_{\mathbf{A},\mathbf{B}} := \{\varphi \in \mathrm{CP}(M_n, M_k) \mid \varphi(A_\nu) = B_\nu, \ \text{for all } \nu = 1, \ldots, N\}.$$

Clearly, the set $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ is convex and closed, but it may or may not be compact. Since the maps $\varphi \in \mathrm{CP}(M_n, M_k)$ are, by definition, linear, without loss of generality one can assume that the set $\{A_1, \ldots, A_N\}$ is linearly independent, otherwise some linear dependence conditions on the output data $\mathbf{B}$ are necessary. On the other hand, since any $\varphi \in \mathrm{CP}(M_n, M_k)$ 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 $A_1, \ldots, A_N, B_1, \ldots, B_N$ are Hermitian. In particular, letting $\mathcal{S}_{\mathbf{A}}$ denote the linear span of $A_1, \ldots, A_N$, it follows that $\mathcal{S}_{\mathbf{A}}$ is a $*$-subspace of M_n, that is, it is a linear subspace stable under taking adjoints, and then, letting $\varphi_{\mathbf{A},\mathbf{B}} \colon \mathcal{S}_{\mathbf{A}} \to M_k$ be the linear map uniquely determined by the conditions

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

it follows that any $\varphi \in \mathrm{CP}(M_n, M_k)$ satisfying the constraints (1.2) should necessarily be an extension of $\varphi_{\mathbf{A},\mathbf{B}}$. Thus, the Interpolation Problem may require certain "positivity" properties of the map $\varphi_{\mathbf{A},\mathbf{B}}$ but the $*$-subspace $\mathcal{S}_{\mathbf{A}}$ may not be linearly generated by $\mathcal{S}_{\mathbf{A}}^+$, the collection of its positive semidefinite matrices or, it may happen that $\mathcal{S}_{\mathbf{A}}$ may contain no nontrivial positive semidefinite matrix at all.

If the $*$-subspace $\mathcal{S}_{\mathbf{A}}$ contains the identity matrix I_n (e.g. if we are interested in solutions φ that are unital, that is, $\varphi(I_n) = I_k$), making it an *operator system* [18], then $\mathcal{S}_{\mathbf{A}}$ is linearly generated by the cone of its positive semidefinite matrices. In this case, there is the celebrated Arveson's Hahn-Banach Type Theorem [3], see the equivalence of (a) and (d) in Theorem 2.6, saying that the Interpolation Problem has a solution if and only if $\varphi_{\mathbf{A},\mathbf{B}}$ has a certain "complete positivity" property. The original proof in [3] of this extension theorem was simplified by R.R. Smith and J.D. Ward [20] who introduced a certain linear functional, that we call the *Smith-Ward functional*, and then reducing the problem to finding positive extensions of it. In the case of the Interpolation Problem, letting $s_{\mathbf{A},\mathbf{B}}$ denote the Smith-Ward linear functional associated to $\varphi_{\mathbf{A},\mathbf{B}}$, see (3.4), one can go further and associate a "density matrix" $D_{\mathbf{A},\mathbf{B}}$, see (3.6), to the Smith-Ward linear functional and then get, see Theorem 3.7, that the solvability of the Interpolation Problem is equivalent with three assertions: firstly, with the complete positivity of $\varphi_{\mathbf{A},\mathbf{B}}$, secondly, with the positivity of the Smith-Ward linear functional $s_{\mathbf{A},\mathbf{B}}$ and, finally, with the fact that the affine space $D_{\mathbf{A},\mathbf{B}} + M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp$ contains positive semidefinite matrices.

On the other hand, a careful inspection of Theorem 3.7 shows that, actually, the Arveson's Hahn-Banach Theorem and the Smith-Ward linear functional $s_{\mathbf{A},\mathbf{B}}$, seem to rather play the role of the hidden catalysts of the "reaction" but do not seem to play the major role. Indeed, the restrictive assumption that $\mathcal{S}_{\mathbf{A}}$ is generated by $\mathcal{S}_{\mathbf{A}}^+$ can be dropped and in Theorem 3.4 we show that the solvability of the Interpolation Problem is equivalent with the fact that the affine subspace $D_{\mathbf{A},\mathbf{B}} + M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp$ contains positive semidefinite matrices, in the full generality. In addition, Theorem 3.4 yields, as a by-product, a parametrisation of the set of all solutions of the Interpolation Problem by the closed convex subset $\mathcal{P}_{\mathbf{A},\mathbf{B}} := \{P \in (M_k \otimes \mathcal{S}_{\mathbf{A}}^\perp)^{\mathrm{h}} \mid P \geq -D_{\mathbf{A},\mathbf{B}}\}$, through an affine isomorphism. In case $\mathcal{S}_{\mathbf{A}}$ is a $*$-subspace congruent to an operator system, then the parameterising convex subset $\mathcal{P}_{\mathbf{A},\mathbf{B}}$ is compact as well.

The density matrix $D_{\mathbf{A},\mathbf{B}}$ plays the major role in our approach to the Interpolation Problem and it is a simple observation, see Remarks 3.6, that the positive semidefiniteness of $D_{\mathbf{A},\mathbf{B}}$ 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 Subsection 2.4 and we provide examples and counter-examples illustrating the complexity of this phenomenon. In addition, in Theorem 2.12 we show that, in case an operator system $\mathcal{S}$ is generated by matrix units, 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, it is the additional assumption that the $*$-subspace is an algebra that ensures the fact that the solvability of the Interpolation Problem is equivalent to the positive definiteness of $D_{\mathbf{A},\mathbf{B}}$, even though exotic cases of $*$-subspaces that are not algebras but when this equivalence happens may occur as well, see Examples 2.10.

In Subsection 3.2 we show that, if the input data $\mathbf{A}$ is orthonormalised with respect to the Hilbert-Schmidt inner product, then the density matrix is easily calculable as $D_{\mathbf{A},\mathbf{B}} = \sum_{\nu=1}^{N} B_\nu^T \otimes A_\nu$ and this considerably simplifies the criterion of solvability of the Interpolation

Problem, see Theorem 3.13. Also, we observe that the Gram-Schmidt orthonormalisation does not affect the other assumptions.

Another important observation on the density matrix $D_{\mathbf{A},\mathbf{B}}$ is that, one might think that it is the Choi matrix [5] 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 Subsection 2.1, we have to use all the matrix units, but the subspace $\mathcal{S}_{\mathbf{A}}$ 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 $\varphi \in \mathrm{CP}(M_n, M_k)$, see Proposition 2.8, we can define a "partial Choi matrix", see (2.29), for linear maps on subspaces.

Finally, in Subsection 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 [7], 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.** For $n \in \mathbb{N}$ let $\{e_i^{(n)}\}_{i=1}^n$ be the canonical basis of $\mathbb{C}^n$. As usually, 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 $\mathbb{C}^k \to \mathbb{C}^n$. For $n, k \in \mathbb{N}$ we consider the matrix units $\{E_{l,i}^{(n,k)} \mid l = 1, \ldots, n, \ i = 1, \ldots, k\} \subset M_{n,k}$ 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 $\varphi \colon M_n \to M_k$ define an $kn \times kn$ matrix Φ_φ by

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

This transformation appears more or less explicitly at J. de Pillis [19], A. Jamiołkowski [11], R.D. Hill [9], and M.D. Choi [5]. In the following we describe more explicitly the transformation $\varphi \mapsto \Phi_\varphi$. We use the lexicographic reindexing of $\{E_{l,i}^{(n,k)} \mid l = 1, \ldots, n, \ i = 1, \ldots, k\}$, more precisely

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

An even more explicit form of this reindexing is the following

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

The formula

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

and its inverse

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

establish a linear and bijective correspondence

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

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

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

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

Let $\varphi : M_n \to M_k$ be a completely positive map. Then, cf. K. Kraus [14] and M.D. Choi [5], there are $n \times k$ matrices $V_1, V_2, \ldots, V_m$ with $m \le nk$ such that

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

The representation (2.8) is called the *Kraus representation* of φ and the matrices $V_1, \ldots, V_m$ are called the *operation elements*. Note that the representation (2.8) of a given completely positive map φ is highly non-unique, not only with respect to its operation elements but also with respect to m, the number of these elements. Concerning the minimal number of the operation elements in the Kraus form representation of completely positive maps on full matrix algebras, the following statement, which is implicit in the original article of M.D. Choi [5], holds.

Proposition 2.1. *Let $\varphi \in \mathrm{CP}(M_n, M_k)$ be a completely positive map and let Φ be its Choi matrix. Then,* $\mathrm{rank}(\Phi)$ *is the minimal number of the operation elements of φ.*

Proof. Let $V = [v_{l,i}]$, with $l = 1, \ldots, n$ and $i = 1, \ldots, k$, be a nontrivial $n \times k$ matrix such that $\varphi(A) = V^* A V$ for all $A \in M_n$. Then, for all $l, m = 1, \ldots, n$ and all $i, j = 1, \ldots, k$, by (2.4) we have

$$(2.9) \qquad \varphi_{(l-1)k+i,(m-1)k+j} = \langle \varphi(E_{l,m}^{(n)})e_j^{(k)}, e_i^{(k)} \rangle = \langle E_{l,m}^{(n)} V e_j^{(k)}, V e_i^{(k)} \rangle = v_{m,j}\overline{v_{l,i}}.$$

We take into account that the reindexing $r = r(l,i) = (l-1)k+i$ is a one-to-one correspondence between $\{r \mid 1 \le r \le nk\}$ and $\{(l,i) \mid 1 \le l \le n, \ 1 \le i \le k\}$, hence (2.9) is equivalent with

$$(2.10) \qquad \varphi_{r,s} = f_s \overline{f_r}, \quad r,s = 1, \ldots, nk,$$

where $f_r = v_{l,i}$ whenever $r = r(l,i) = (l-1)k+i$. This proves that the Choi matrix Φ has rank 1.

From the particular case proved before, since the correspondence between Choi matrices and completely positive maps is bijective and affine, it follows that, if φ has the representation (2.8), $\mathrm{rank}(\Phi) \le m$. On the other hand, if $m = \mathrm{rank}(\Phi)$, then $\Phi = \Phi_1 + \Phi_2 + \cdots + \Phi_m$ with positive matrices Φ_j, $\mathrm{rank}(\Phi_j) = 1$ for all $j = 1, \ldots, m$. Then, from the particular case proved before, for each $j = 1, \ldots, m$, it follows that $\Phi_j(A) = V_j^* A V_j$ for some $V_j \in M_{k,n}$ and all $A \in M_n$, hence Φ has the Kraus representation (2.8). $\qquad \square$

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. 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 $\mathcal{S}^{\mathrm{h}}$ of all its Hermitian matrices. Also, $\mathcal{S}^+ = \{A \in \mathcal{S} \mid A \geq 0\}$ is a cone in $\mathcal{S}^{\mathrm{h}}$ but, in general, $\mathcal{S}^+$ may fail to linearly generate $\mathcal{S}^{\mathrm{h}}$. Recall [18] 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 characterisations 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 2.2. *Given two matrices* $A, B \in M_m^+$, *we have* $B \leq \alpha A$, *for some some* $\alpha > 0$, *if and only if* $\mathrm{Ran}(B) \subseteq \mathrm{Ran}(A)$.

Proof. A folklore result in operator theory, e.g. see [6], says that for two matrices $A, B \in M_m$, the inequality $BB^* \leq \alpha AA^*$, for some $\alpha > 0$, is equivalent with $\mathrm{Ran}(B) \subseteq \mathrm{Ran}(A)$. Consequently, if $A, B \in M_m^+$ then $B \leq A$ if and only if $\mathrm{Ran}(B^{1/2}) \subseteq \mathrm{Ran}(A^{1/2})$. From here the statement follows since we have $\mathrm{Ran}(P) = \mathrm{Ran}(P^{1/2})$ for any positive semidefinite matrix P. $\square$

Proposition 2.3. *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* $B \in \mathcal{S}^{\mathrm{h}}$ *we have* $B \leq \alpha A$ *for some* $\alpha > 0$.
   (iii) *For any* $B \in \mathcal{S}^{\mathrm{h}}$ *there exists* $A \in \mathcal{S}^+$ *with* $B \leq A$.
   (iv) *There exists* $T \in M_m$ *a matrix of rank* r, *with* $\mathrm{Ran}(T) = \mathbb{C}^r \oplus 0 \subseteq M_m$, *and an operator system* $\mathcal{T} \subseteq M_r$ *such that*

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

   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 2.2, $\mathrm{Ran}(B) \not\subseteq \mathrm{Ran}(A)$ hence, $\mathrm{Ran}(A)$ is a proper subspace of $\mathrm{Ran}(A) + \mathrm{Ran}(B)$. Since $A, B \leq A + B$, again by Lemma 2.2 it follows $\mathrm{Ran}(B) + \mathrm{Ran}(A) \subseteq \mathrm{Ran}(A + B)$. But then, $A + B \in \mathcal{S}^+$ has bigger rank than A, which contradicts the choice of A.

Let now $B \in \mathcal{S}^{\mathrm{h}}$ 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 $\mathcal{S}^{\mathrm{h}}$ is (real) linearly generated by $\mathcal{S}^+$. To see this, let $B \in \mathcal{S}^{\mathrm{h}}$ 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 $B \in \mathcal{S}^\mathrm{h}$ there exists $\alpha > 0$ such that $B \leq \alpha A$. By Lemma 2.2, it follows that for any $B \in \mathcal{S}^+$ we have $\mathrm{Ran}(B) \subseteq \mathrm{Ran}(A)$ hence, since $\mathcal{S}$ is linearly generated by $\mathcal{S}^+$, it follows that for any $B \in \mathcal{S}$ we have $\mathrm{Ran}(B) \subseteq \mathrm{Ran}(A)$, in particular, $\mathrm{Ran}(A)$ reduces B and

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

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

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

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

$$\mathcal{T} = V \mathcal{T}_0 V^* \text{ and } T = V A^{1/2}$$

the conclusion follows.

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

Corollary 2.4. *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 $\mathcal{S}^+$. $\qquad\square$

In the following we will use a particular case of the celebrated theorem of L. Kantorovich [13], see also Theorem I.30 in [2], of Hahn-Banach type.

Lemma 2.5. *Let $\mathcal{S}$ be an $*$-subspace of M_m that is linearly generated by $\mathcal{S}^+$, and let $f \colon \mathcal{S} \to \mathbb{C}$ 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 $\widetilde{f} \colon M_m \to \mathbb{C}$ that extends f.*

Proof. Briefly, the idea is to consider the $\mathbb{R}$-linear functional $f_\mathrm{h} = f|\mathcal{S}^\mathrm{h}$ and note that f_h is positive. By Proposition 2.3, there exists $A \in \mathcal{S}^+$ such that for all $B \in \mathcal{S}^\mathrm{h}$ there exists $\alpha > 0$ with $B \leq \alpha A$. By Lemma 2.2, we have $\mathrm{Ran}(B) \subseteq \mathrm{Ran}(A)$ for all $B \in \mathcal{S}^\mathrm{h}$. Let $p \colon \mathcal{B}(\mathrm{Ran}(A))^\mathrm{h} \to \mathbb{R}$ be defined by

(2.12) $$p(C) = \inf\{f_\mathrm{h}(B) \mid C \leq B \in \mathcal{S}^\mathrm{h}\}, \quad C \in \mathcal{B}(\mathrm{Ran}(A))^\mathrm{h}.$$

Then p is a sublinear functional on the $\mathbb{R}$-linear space $\mathcal{B}(\mathrm{Ran}(A))^\mathrm{h}$ and $f(B) = p(B)$ for all $B \in \mathcal{S}^\mathrm{h}$. By the Hahn-Banach Theorem, there exists a linear functional $g \colon \mathcal{B}(\mathrm{Ran}(A))^\mathrm{h} \to \mathbb{R}$ that extends f_h and such that $g(B) \leq p(B)$ for all $B \in \mathcal{B}(\mathrm{Ran}(A))^\mathrm{h}$. Then, for any $B \in M_m^+$, since $-B \leq 0$ it follows $-g(B) = g(-B) \leq p(-B) \leq f_\mathrm{h}(0) = 0$, hence $g(B) \geq 0$. Then, let $\widetilde{f}$ be the canonical extension of g to $\mathcal{B}(\mathrm{Ran}(A)) = \mathcal{B}(\mathrm{Ran}(A))^\mathrm{h} + i\mathcal{B}(\mathrm{Ran}(A))^\mathrm{h}$, in the usual

way, and finally extend $\widetilde{f}$ to M_m by letting $\widetilde{f}(B) = \widetilde{f}(P_{\mathrm{Ran}(A)}B|\mathrm{Ran}(A))$ for all $B \in M_m$, where $P_{\mathrm{Ran}(A)}$ denotes the orthogonal projection of $\mathbb{C}^m$ onto $\mathrm{Ran}(A)$. $\square$

2.3. **The Smith-Ward Functional.** In the following we recall a technical concept introduced by R.R. Smith and J.D. Ward, cf. the proof of Theorem 2.1 in [20], and there used to provide another proof to the Arveson's Hahn-Banach Theorem [3] for completely positive maps, see also Chapter 6 in [18]. 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 2.3. Thus, a linear map $\varphi \colon \mathcal{S} \to M_k$, 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 $\varphi_m = I_m \otimes \varphi \colon M_m \otimes \mathcal{S} \to M_m \otimes M_k$, 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

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

Then, φ is called *m-positive* if φ_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 $\varphi \colon \mathcal{S} \to M_k$, where $\mathcal{S} \subseteq M_n$ is some linear subspace, one associates a linear functional $s_\varphi \colon M_k(\mathcal{S}) \to \mathbb{C}$, via the canonical identification of $M_k(\mathcal{S}) \simeq M_k \otimes \mathcal{S}$, by

$$(2.13) \qquad s_\varphi([A_{i,j}]_{i,j=1}^k) = \sum_{i,j=1}^k \langle \varphi(A_{i,j})e_j^{(k)}, e_i^{(k)} \rangle_{\mathbb{C}^k}$$

$$= \langle (I_k \otimes \varphi([A_{i,j}]_{i,j=1}^k))e^{(k)}, e^{(k)} \rangle_{\mathbb{C}^{k^2}}$$

$$= \langle [\varphi(A_{i,j})]_{i,j=1}^k e^{(k)}, e^{(k)} \rangle_{\mathbb{C}^{k^2}}$$

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

$$(2.14) \qquad e^{(k)} = e_1^{(k)} \oplus \cdots \oplus e_k^{(k)} \in \mathbb{C}^{k^2} = \mathbb{C}^k \oplus \cdots \oplus \mathbb{C}^k.$$

The formula (2.13) establishes a linear isomorphism

$$(2.15) \qquad \mathcal{B}(\mathcal{S}, M_k) \ni \varphi \mapsto s_\varphi \in (M_k \otimes \mathcal{S})^* \simeq \mathcal{B}(M_k \otimes \mathcal{S}, \mathbb{C}),$$

with the inverse transformation

$$(2.16) \qquad (M_k \otimes \mathcal{S})^* \simeq \mathcal{B}(M_k \otimes \mathcal{S}, \mathbb{C}) \ni s \mapsto \varphi_s \in \mathcal{B}(\mathcal{S}, M_k)$$

given by the formula

$$(2.17) \qquad \varphi_s(A) = [s(E_{i,j}^{(k)} \otimes A)]_{i,j=1}^k, \quad A \in \mathcal{S}.$$

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 [3], while the equivalence of (a), (b), and (d) is essentially due to R.R. Smith and J.D. Ward [20] as another 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 $\varphi\colon \mathcal{S} \to M_k$ be a linear map. The following assertions are equivalent:*

(a) *φ is completely positive.*
(b) *φ is k-positive.*
(c) *s_φ is a positive functional.*
(d) *There exists $\widetilde{\varphi} \in \mathrm{CP}(M_k, M_n)$ that extends φ.*

Proof. Clearly (a) implies (b), the fact that (b) implies (c) follows from the definition of s_φ as in (2.13), while (d) implies (a) is clear as well. The only nontrivial part is (c) implies (d). Briefly, following the proofs of Theorem 6.1 and Theorem 6.2 in [18], the idea is to use Kantorovich's Theorem as in Lemma 2.5 in order to extend s_φ to a positive functional $\widetilde{s}$ on $M_k \otimes M_n \simeq M_k(M_n) \simeq M_{kn}$ then, in view of (2.17), let $\widetilde{\varphi}\colon M_k \to M_n$ be defined by

$$(2.18) \qquad \widetilde{\varphi}(A) = [\widetilde{s}(E_{i,j}^{(k)} \otimes A)]_{i,j=1}^k, \quad A \in M_n,$$

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

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

we have

$$\sum_{i,j=1}^m \langle \widetilde{\varphi}(A_i^* A_j) h_j, h_i \rangle_{\mathbb{C}^k} = \sum_{i,j=1}^m \sum_{l,p=1}^k \lambda_{j,l} \overline{\lambda}_{i,p} \langle \widetilde{\varphi}(A_i^* A_j) e_l^{(k)}, e_p^{(k)} \rangle_{\mathbb{C}^k}$$

$$= \sum_{i,j=1}^m \sum_{l,p=1}^k \lambda_{j,l} \overline{\lambda}_{i,p} \widetilde{s}(A_i^* A_j \otimes E_{p,l}^{(k)})$$

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

$$= \sum_{i,j=1}^m \widetilde{s}(A_i^* A_j \otimes B_i^* B_j)$$

$$= \widetilde{s}((\sum_{i=1}^m A_i \otimes B_i)^* (\sum_{j=1}^m A_j \otimes B_j)) \geq 0. \qquad \square$$

Actually, once the facts described in Theorem 2.6 are settled, it is easy to observe that (2.13) *and* (2.17) *establish an affine and order preserving bijection between the cone* $\mathrm{CP}(\mathcal{S}, M_k)$ *and the cone* $\{s\colon M_k(\mathcal{S}) \to \mathbb{C} \mid s \text{ linear and positive}\}$.

2.4. **The Density Matrix.** We consider M_m as a Hilbert space with the Hilbert-Schmidt inner product, that is, $\langle C, D \rangle_{\mathrm{HS}} = \mathrm{tr}(D^*C)$, for all $C, D \in M_m$. Thus, to any linear functional $s \colon M_m \to \mathbb{C}$, 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

$$(2.19) \qquad\qquad s(C) = \mathrm{tr}(D_s^*C), \quad C \in M_m.$$

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 $\mathrm{tr}(D_sC) = \mathrm{tr}(C^{1/2}D_sC^{1/2}) \geq 0$. Conversely, if $\mathrm{tr}(D_sC) \geq 0$ for all positive semidefinite $m \times m$ matrix C, then for any vector v of length m we have $0 \leq \mathrm{tr}(D_svv^*) = \mathrm{tr}(v^*D_sv) = v^*D_sv$, 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.

On the other hand, since the correspondence between linear maps $\varphi \colon M_n \to M_k$ and Choi matrices $\Phi_\varphi \in M_{kn}$ is a linear isomorphism and, via the Smith-Ward linear functional s_φ, the correspondence between φ and the density matrix D_{s_φ} is a conjugate linear isomorphism, it is natural to ask for an explicit relation between the Choi matrix Φ_φ and D_{s_φ}. 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

$$(2.20) \qquad\qquad U e^{(kn)}_{(i-1)n+l} = e^{(kn)}_{(l-1)k+i}.$$

It is clear that U is a unitary operator $\mathbb{C}^{kn} \to \mathbb{C}^{kn}$, 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 $\overline{X}$.

Proposition 2.8. *For any linear map $\varphi \colon M_n \to M_k$ and letting Φ denote its Choi matrix, cf. (2.1), the density matrix D associated to the Smith-Ward linear functional s_φ, cf. (2.19) and (2.13), is*

$$(2.21) \qquad\qquad D = U^*\overline{\Phi}U,$$

where U is the canonical shuffle unitary operator defined at (2.20).

Proof. We first note that $\{E^{(k)}_{i,j} \otimes E^{(n)}_{l,m} \mid i,j = 1, \dots, k, \ l,m = 1, \dots, n\}$ 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

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

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

$$s_\varphi(E^{(k)}_{i,j} \otimes E^{(n)}_{l,m}) = s_\varphi(E^{(kn)}_{(i-1)n+l,(j-1)n+m})$$

$$(2.22) \qquad\qquad = \mathrm{tr}(D^*E^{(kn)}_{(i-1)n+l,(j-1)n+m}) = \overline{d}_{(i-1)n+l,(j-1)n+m},$$

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

$$(2.23) \qquad s_\varphi(E_{i,j}^{(k)} \otimes E_{l,m}^{(n)}) = \langle \varphi(E_{l,m}^{(n)}) e_j^{(k)}, e_i^{(k)} \rangle_{\mathbb{C}^k} = \varphi_{(l-1)k+i,(m-1)k+j}.$$

Therefore, in view of (2.22), (2.23) we have

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

hence, taking into account of the definition of the canonical shuffle operator U as in (2.20), the equality in (2.21) follows. $\qquad \square$

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

$$(2.24) \qquad s(C) = \operatorname{tr}(D_s^* C), \quad C \in \mathcal{S},$$

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. Clearly, 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 2.9. (1) If the $\mathcal{S}$ is a $*$-subspace of M_n and the linear functional $s \colon \mathcal{S} \to \mathbb{C}$ 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

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

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 $s \colon \mathcal{S} \to \mathbb{C}$, its density matrix D is positive semidefinte. Indeed, in this case $D = D_+ - D_-$ with $D_\pm \in \mathcal{S}^+$ and $D_+ D_- = 0$ hence $0 \le s(D_-) = \operatorname{tr}(DD_-) = -\operatorname{tr}(D_-^2)$ hence $D_- = 0$ and consequently $D \in \mathcal{S}^+$.

Examples 2.10. (1) We consider the following operator system $\mathcal{S}$ in M_3

$$(2.25) \qquad \mathcal{S} = \left\{ C = \begin{bmatrix} a & 0 & b \\ 0 & a & 0 \\ c & 0 & d \end{bmatrix} \mid a, b, c, d \in \mathbb{C} \right\},$$

and note that $\mathcal{S}^+$ consists on those matrices C as in (2.25) with $c = \overline{b}$, $a, d \geq 0$, 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 (2.25), $c = \overline{b}$, $a, d \geq 0$, and $|b|^2 \leq ad$, we have

$$\operatorname{tr}(DC) = a + \sqrt{2}\,\overline{b} + a + \sqrt{2}\,b + d = 2a + d + 2\sqrt{2}\operatorname{Re} b$$
$$\geq 2a + d - 2\sqrt{2}|b| \geq 2a + d - 2\sqrt{2}\sqrt{ad} = (\sqrt{2a} - \sqrt{d})^2 \geq 0,$$

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

(2) In M_2 we consider the Pauli matrices

$$(2.26) \qquad \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

that makes an orthogonal basis of M_2 with respect to the Hilbert-Schmidt inner product. We consider $\mathcal{S}$ the linear span of σ_0, σ_1, and σ_2, more precisely,

$$(2.27) \qquad \mathcal{S} = \{C = \begin{bmatrix} \alpha & \beta \\ \gamma & \alpha \end{bmatrix} \mid \alpha, \beta, \gamma \in \mathbb{C}\}.$$

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 $\operatorname{tr}(D^*C) \geq 0$ for all $C \in \mathcal{S}^+$.

To this end, note that a matrix C as in (2.27) is positive semidefinite if and only if $\gamma = \overline{\beta}$, $\alpha \geq 0$, and $|\beta|^2 \leq \alpha^2$. Let $D \in \mathcal{S}$, that is,

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

such that $\operatorname{tr}(D^*C) \geq 0$ for all $C \in \mathcal{S}^+$. From Remark 2.9 it follows that D is Hermitian, hence a is real and $c = \overline{b}$, and the condition $\operatorname{tr}(D^*C) \geq 0$ can be equivalently written as

$$(2.28) \qquad a\alpha + \operatorname{Re}(\overline{\beta}b) \geq 0 \text{ whenever } \alpha \geq 0 \text{ and } |\beta|^2 \leq \alpha^2.$$

Letting $\beta = 0$ implies that $a \geq 0$. We prove that $|b|^2 \geq a^2$. If $a = 0$ then from (2.28) it follows that $b = 0$. If $a > 0$ and $|b|^2 > a^2$ then letting $\alpha = a$ and $\beta = -a|b|/\overline{b}$, we obtain $0 \leq a\alpha + \operatorname{Re}(\overline{\beta}b) = a^2 - a|b| = a(a - |b|) < 0$, a contradiction. Hence $|b|^2 \geq a^2$ must hold, and we have proven that D is positive semidefinite.

The concept of density matrices associated to linear functionals on $*$-subspaces opens the possibility of generalising 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 2.8 we can proceed as follows. First consider the Smith-Ward functional s_φ defined as in (2.13), then consider the density matrix D_φ associated to s_φ as in (2.24), and finally define Φ_φ by

$$(2.29) \qquad \Phi_\varphi = U\,\overline{D_\varphi}\,U^*,$$

where the bar denotes the entrywise complex conjugation and U denotes the canonical shuffle unitary operator as in (2.20). Clearly Φ_φ is an $kn \times kn$ matrix and, in case $\varphi \in \mathrm{CP}(\mathcal{S}, M_k)$, the Choi matrix C_φ defined as in (2.29) 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 Φ_φ is positive semidefinite, then $\varphi \in \mathrm{CP}(\mathcal{S}, M_k)$.

2.5. **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 $S \subseteq \{1, \ldots, m\}^2$ such that $\mathcal{S} = \mathrm{Lin}\{E_s^{(m)} \mid s \in S\}$.

Remarks 2.11. In the following we use the interpretation of subsets $S \subseteq \{1, \ldots, m\}^2$ as relations on the set $\{1, \ldots, m\}$. Let S be a relation on $\{1, \ldots, m\}$ and let $\mathcal{S} = \mathrm{Lin}\{E_s^{(m)} \mid s \in S\}$ be the linear subspace in M_m generated by the matrix unit 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 unital $*$-subalgebra of M_m if and only if S is an equivalence relation.

Theorem 2.12. *Let $\mathcal{S}$ be an operator system in M_m linearly generated by matrix units. The following assertions are equivalent:*

(a) *Any positive linear functional $s\colon \mathcal{S} \to \mathbb{C}$ has a positive semidefinite density matrix.*

(b) *$\mathcal{S}$ is an algebra (and hence a unital $*$-subalgebra of M_m).*

Proof. (a)$\Rightarrow$(b). We divide the proof in three steps:

Step 1. 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 2.9.(2), there is nothing to prove.

Step 2. We consider $m = 3$ so let $\mathcal{S}$ be an operator system in M_3 that is linearly generated by a reflexive and symmetric relation $S \subseteq \{1, 2, 3\}^2$. Then S necessarily contains all the diagonal $S_\mathrm{d} = \{(1, 1), (2, 2), (3, 3)\}$. 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. Thus, we are left only with the investigation of the case when S has exactly 7 elements, and these are the cases when $S = S_\mathrm{d} \cup \{(1, 2), (2, 1), (1, 3), (3, 1)\}$, $S = S_\mathrm{d} \cup \{(1, 2), (2, 1), (3, 2), (2, 3)\}$, $S = S_\mathrm{d} \cup \{(2, 3), (3, 2), (1, 3), (3, 1)\}$. 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 $\mathcal{S} = \mathrm{Lin}\, S$, 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

$$(2.30) \qquad \mathcal{S} = \left\{ C = \begin{bmatrix} a & b & c \\ f & d & 0 \\ g & 0 & e \end{bmatrix} \mid a, b, c, d, e, f, g \in \mathbb{C} \right\},$$

and that $\mathcal{S}^+$ is the collection of all matrices C as in (2.30) subject to the following conditions

(2.31) $a \geq 0, \ d \geq 0, \ e \geq 0, f = \overline{b}, g = \overline{c}, \ |b|^2 \leq ad, \ |c|^2 \leq ae, \ |b|^2 e + |c|^2 d \leq ade.$

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

(2.32)
$$D_\rho = \begin{bmatrix} 1 & \rho & \rho \\ \rho & 1 & 0 \\ \rho & 0 & 1 \end{bmatrix}.$$

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

We prove that the corresponding functional $s_\rho = \mathrm{tr}(D_\rho \cdot)$ 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 (2.30), the conditions (2.31) must hold. Then

$$s_\rho(C) = \mathrm{tr}(D_\rho C) = a + d + e + 2\rho \, \mathrm{Re}(b + c)$$
$$\geq a + d + e - 2\rho(|b| + |c|)$$

and, taking into account that $|b| + |c|$ has its maximal value $\sqrt{a(e + d)}$ when the constraints (2.31) hold, it follows that

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

Step 3. Assume now that $m > 3$ and assume that $\mathcal{S}$ is an operator system in M_m that is not an algebra. By Remark 2.11.(2), there exist distinct $i, j, l \in \{1, \ldots, m\}$ 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_ρ as in (2.32) and let $\widetilde{D}_\rho = D_\rho \oplus 0 \in M_m$. From what has been proven in Step 3 it follows that the functional $s_\rho = \mathrm{tr}(\widetilde{D}_\rho \cdot)$ on M_m is positive but its density matrix $\widetilde{D}_\rho$ is not positive semidefinite.

(b)$\Rightarrow$(a). This is a consequence of Remark 2.9.(2). $\square$

3. Main Results

3.1. **The General Case.** Let now $A_1, \ldots, A_N \in M_n$ and $B_1, \ldots, B_N \in M_k$ be the given interpolation data with respect to the Interpolation Problem, see the Introduction. We recall the notation $\mathbf{A} = (A_1, \ldots, A_N)$, called the *input data* and, similarly, $\mathbf{B} = (B_1, \ldots, B_N)$, called the *output data*. Since we are looking for $\varphi \in \mathrm{CP}(M_n, M_k)$, hence for Hermitian maps $\varphi \colon M_n \to M_k$, such that the interpolation condition holds

(3.1) $\varphi(A_\nu) = B_\nu, \ \text{for all } \nu = 1, \ldots, N,$

without loss of generality we can assume that all A_ν and all B_ν 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 $A_1, \ldots, A_N$ are linearly independent, otherwise some linearly dependence consistency conditions on $B_1, \ldots, B_N$

should be imposed. On the other hand, since the required maps φ should be linear, the constraint (3.1) actually determines φ on the space

$$(3.2) \qquad \mathcal{S}_{\mathbf{A}} = \mathrm{Lin}\{A_1, \ldots, A_N\},$$

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

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

Thus, $\mathcal{S}_{\mathbf{A}}$ is $*$-subspace of M_n for which $A_1, \ldots, A_N$ is a linear basis. Having in mind the approach of the Interpolation Problema through the Arveson's Hahn-Banach Theorem and Smith-Ward linear functional, $\mathcal{S}_{\mathbf{A}}$ might be required to be linearly generated by $\mathcal{S}_{\mathbf{A}}^+$. Thus, 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) $\mathcal{S}_{\mathbf{A}}$ *is linearly generated by* $\mathcal{S}_{\mathbf{A}}^+$.

Remark 3.1. Recalling the definition of $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ as in (1.3), the set of solutions of the Interpolation Problem, observe that $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ is convex and closed. If $\mathcal{S}_{\mathbf{A}}$ contains a positive definite matrix of rank n, in particular, if $\mathcal{S}_{\mathbf{A}}$ is an operator system, then $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ is bounded as well, hence compact. Indeed, if $\mathcal{S}_{\mathbf{A}}$ is an operator system, this follows from the fact, e.g. see Proposition 3.6 in [18], that $\|\varphi\| = \|\varphi(I_n)\|$ and, since $I_n \in \mathcal{S}_{\mathbf{A}}$, the positive semidefinite matrix $\varphi(I_n)$ is fixed and independent of $\varphi \in \mathcal{C}_{\mathbf{A},\mathbf{B}}$. The general case follows now by Proposition 2.3. However, the same Proposition 2.3 shows that assuming that $\mathcal{S}_{\mathbf{A}}$ is generated by $\mathcal{S}_{\mathbf{A}}^+$ is not sufficient for the compactness of $\mathcal{C}_{\mathbf{A},\mathbf{B}}$.

In order to approach the Interpolation Problem, it is natural to associate a linear map $\varphi_{\mathbf{A},\mathbf{B}} \colon \mathcal{S}_{\mathbf{A}} \to M_k$ to the data $\mathbf{A}$ and $\mathbf{B}$ by letting

$$(3.3) \qquad \varphi_{\mathbf{A},\mathbf{B}}(A_\nu) = B_\nu, \quad \nu = 1, \ldots, N,$$

and then uniquely extending it by linearity to the whole $*$-subspace $\mathcal{S}_{\mathbf{A}}$. Then, having in mind the Smith-Ward linear functional (2.13), let

$$(3.4) \qquad s_{\mathbf{A},\mathbf{B}}(E_{i,j}^{(k)} \otimes A_\nu) = \langle B_\nu e_j^{(k)}, e_i^{(k)} \rangle_{\mathbb{C}^k} = b_{i,j,\nu}, \quad i,j = 1, \ldots, N, \ \nu = 1, \ldots, N,$$

where

$$(3.5) \qquad B_\nu = \sum_{i,j=1}^{k} b_{i,j,\nu} E_{i,j}^{(k)}, \quad \nu = 1, \ldots, N.$$

Since $\{E_{i,j}^{(k)} \otimes A_\nu \mid i,j = 1, \ldots k, \ \nu = 1, \ldots, N\}$ is a basis for $M_k \otimes \mathcal{S}_{\mathbf{A}}$, it follows that $s_{\mathbf{A},\mathbf{B}}$ admits a unique extension to a linear functional $s_{\mathbf{A},\mathbf{B}}$ on $M_k(\mathcal{S}_{\mathbf{A}})$. Note that, with respect to the transformations (2.13) and (2.16), the functional $s_{\mathbf{A},\mathbf{B}}$ corresponds to the map $\varphi_{\mathbf{A},\mathbf{B}}$, and vice-versa.

To the linear functional $s_{\mathbf{A},\mathbf{B}}$ one also uniquely associates its density matrix $D_{\mathbf{A},\mathbf{B}}$ as in (2.24), more precisely,

$$(3.6) \qquad s_{\mathbf{A},\mathbf{B}}(C) = \mathrm{tr}(D_{\mathbf{A},\mathbf{B}}^* C), \quad C \in \mathcal{S}_{\mathbf{A}},$$

that can be explicitly calculated in terms of input-output data $\mathbf{A}$ and $\mathbf{B}$, as follows.

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

$$(3.7) \qquad D_{\mathbf{A},\mathbf{B}} = \sum_{\nu=1}^{N} \sum_{i,j=1}^{k} d_{i,j,\nu} E_{i,j}^{(k)} \otimes A_\nu,$$

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

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

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 $\{E_{i,j}^{(k)} \otimes A_\nu \mid i, j = 1, \ldots, k, \ \nu = 1, \ldots, N\}$ as in (3.7), so we only have to show that (3.8) holds. To this end, note that

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

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

$$b_{i,j,\nu} = s_{\mathbf{A},\mathbf{B}}(E_{i,j}^{(k)} \otimes A_\nu) = \operatorname{tr}(D_{\mathbf{A},\mathbf{B}}^* (E_{i,j}^{(k)} \otimes A_\nu))$$

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

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

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

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

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

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

Lemma 3.3. *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*

$$(3.9) \qquad \mathcal{S}^\perp = \{E \in M_n \mid \operatorname{tr}(C^* E) = 0, \ \text{for all } C \in \mathcal{S}\}.$$

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 $\operatorname{tr}(E^*C) = 0$ for all $C \in \mathcal{S}$. Then, $0 = \overline{\operatorname{tr}(E^*C)} = \operatorname{tr}(C^*E) = \operatorname{tr}(EC^*) = \operatorname{tr}((E^*)^*C^*)$ 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, $\dim((M_k \otimes \mathcal{S})^\perp) = k^2 n^2 - k^2 \dim(\mathcal{S}) = k^2(n^2 - \dim(\mathcal{S})) = \dim(M_k \otimes \mathcal{S}^\perp)$, 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). $\square$

Theorem 3.4. *Let the data* $A_1, \ldots, A_N \in M_n$ *and* $B_1, \ldots, B_N \in M_k$ *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* (2.24). *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* (3.9).

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* $\nu = 1, \ldots, N$.

(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 $\varphi \in \operatorname{CP}(M_n\, M_k)$ be such that $\varphi(A_\nu) = B_\nu$ for all $\nu = 1, \ldots, N$, hence φ extends the linear map $\varphi_{\mathbf{A},\mathbf{B}}$, and let $s_\varphi \colon M_k(M_n) \to \mathbb{C}$ be the Smith-Ward linear functional associated to φ as in (2.13). Since φ is completely positive, it follows that s_φ is positive. Further, let $D_\varphi \in M_{kn}$ be the density matrix of s_φ, cf. (2.19), hence, by Remark 2.7, D_φ is positive semidefinite. On the other hand, since φ extends $\varphi_{\mathbf{A},\mathbf{B}}$, it follows that s_φ 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

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

hence, letting $s \colon M_{kn} \to \mathbb{C}$ 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 $\varphi_s \colon M_n \to M_k$ be the linear map associated to s as in (2.17). Then φ is completely positive and extends $\varphi_{\mathbf{A},\mathbf{B}}$. $\square$

Corollary 3.5. *Under the assumptions and the notation of Theorem 3.4, suppose that one (hence both) of the equivalent conditions* (i) *and* (ii) *holds. Then, the formula*

$$(3.10) \qquad \varphi(A) = \left[\operatorname{tr}(D_{\mathbf{A},\mathbf{B}} + P)(E_{i,j}^{(k)} \otimes A)\right]_{i,j=1}^k, \quad A \in M_n,$$

establishes an affine isomorphism between the closed convex sets

$$(3.11) \qquad \mathcal{C}_{\mathbf{A},\mathbf{B}} := \{\varphi \in \operatorname{CP}(M_n, M_k) \mid \varphi(A_\nu) = B_\nu, \text{ for all } \nu = 1, \ldots, N\},$$

and

$$(3.12) \qquad \mathcal{P}_{\mathbf{A},\mathbf{B}} := \{P \in (M_k \otimes \mathcal{S}_{\mathbf{A}}^{\perp})^{\mathrm{h}} \mid P \geq -D_{\mathbf{A},\mathbf{B}}\}.$$

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 (3.10) establishes an affine isomorphism between these two convex sets follows, on the one hand, from the affine isomorphism properties of the Smith-Ward functional and of the density matrix and, on other hand, from the proof of Theorem 3.4. $\qquad \square$

Remarks 3.6. Let the assumptions and the notation of Theorem 3.4 hold.

(1) In order for the set $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ to be nonempty, a necessary condition is, clearly, that for arbitrary $\nu = 1, \dots, N$, if A_ν is semidefinite, then B_ν is semidefinite of the same type.

(2) If the density matrix $D_{\mathbf{A},\mathbf{B}}$ is positive semidefinite, as a consequence of Corollary 3.5, the set $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ is nonempty, more precisely, the map $\varphi \colon M_n \to M_k$ defined by

$$(3.13) \qquad \varphi(A) = \left[\mathrm{tr}(D_{\mathbf{A},\mathbf{B}}(E_{i,j}^{(k)} \otimes A))\right]_{i,j=1}^n, \quad A \in M_n,$$

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 2.10.

(3) According to Corollary 3.2 in [16], for any $A \in M_n^+$ and $B \in M_k^+$ there exists $\varphi \in \mathrm{CP}(M_n, M_k)$ 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 $\mathcal{S}_{\mathbf{A}}$ is generated by its positive cone $\mathcal{S}_{\mathbf{A}}^+$. This assumption, for example, becomes natural if we are looking for solutions φ of the Interpolation Problem that are unital, that is, $\varphi(I_n) = I_k$, or if we assume that the data $\mathbf{A}$ and $\mathcal{B}$ 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 A. Jenčová, cf. Theorem 1 in [12], and by T. Heinosaari, M.A. Jivulescu, D. Reeb, M.M. Wolf, cf. Theorem 4 and Corollary 2 in [8] (our Corollary 2.4 and Corollary 2 in [8] explains that the two cited theorems are actually equivalent).

Theorem 3.7. *With the assumptions and the notation as in Theorem 3.4 assume, in addition, that* (a3) *holds as well. The following assertions are equivalent:*

(1) *There exists $\varphi \in \mathrm{CP}(M_n \, M_k)$ 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 $s_{\mathbf{A},\mathbf{B}} \colon M_k \otimes \mathcal{S}_{\mathbf{A}} \to \mathbb{C}$ defined by* (3.4) *is positive.*

(4) *The affine space $D_{\mathbf{A},\mathbf{B}} + M_k \otimes \mathcal{S}_{\mathbf{A}}^{\perp}$ contains at least one positive semidefinite matrix.*

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

(2)⇒(3). Assume that $\varphi_{\mathbf{A},\mathbf{B}}$ is k-positive. With notation as in (2.14), a moment of thought shows that, for each $i, j = 1, \ldots, N$ and each $\nu = 1, \ldots, N$, we have

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

hence

$$(3.14) \qquad \langle (I_k \otimes \varphi_{\mathbf{A},\mathbf{B}})(C) e^{(k)}, e^{(k)} \rangle_{\mathbb{C}^{k^2}} = s_{\mathbf{A},\mathbf{B}}(C), \quad C \in M_k \otimes \mathcal{S}_{\mathbf{A}},$$

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

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

(1)⇔(4). Proven in Theorem 3.4 $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Remark 3.8. Under the assumptions and notation as in Theorem 3.7, if $\mathcal{S}_{\mathbf{A}}$ 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 3.5, is convex and compact as well.

Corollary 3.9. *If the $*$-subspace $\mathcal{S}_{\mathbf{A}}$ is an algebra, then the set $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ is nonempty if and only if $D_{\mathbf{A},\mathbf{B}}$ is positive semidefinite, more precisely, in this case (3.13) provides a solution $\varphi \in \mathcal{C}_{\mathbf{A},\mathbf{B}}$ of the Interpolation Problem.*

Proof. This is a consequence of Theorem 3.7, the second statement of Remark 2.9, and the second statement of Remark 3.6. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Example 2.10.(2) shows that the statement in the previous corollary may be true without the assumption that the $*$-space $\mathcal{S}_{\mathbf{A}}$ is an algebra.

Remark 3.10. *Trace Preserving.* Recall that a linear map $\varphi \colon M_n \to M_k$ is *trace preserving* if $\operatorname{tr}(\varphi(A)) = \operatorname{tr}(A)$ for all $A \in M_n$. With the notation as in Theorem 3.4, let

$$(3.15) \qquad \mathcal{Q}_{\mathbf{A},\mathbf{B}} := \{ \varphi \in \mathcal{C}_{\mathbf{A},\mathbf{B}} \mid \varphi \text{ is trace preserving} \},$$

and we want to determine, with respect to the affine isomorphism established in Corollary 3.5, how the corresponding parameterising subset $\mathcal{P}_{\mathbf{A},\mathbf{B}}$ can be singled out and, implicitly, to get a characterisation of the solvability of the Interpolation Problem for quantum channels. So let $P = [p_{(i,l),(j,m)}]$ be an arbitrary matrix in $\mathcal{P}_{\mathbf{A},\mathbf{B}}$, where $(i, l) = (i-1)n + l$ and $(j, m) = (j-1)n + m$, for $i, j = 1, \ldots, k$ and $l, m = 1, \ldots, n$, 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 (3.10), a map $\varphi \in \mathcal{C}_{\mathbf{A},\mathbf{B}}$ is trace invariant if and only if

$$(3.16) \qquad \operatorname{tr}(\varphi(E_{l,m}^{(n)})) = \operatorname{tr}(E_{l,m}^{(n)}) = \delta_{l,m}, \quad l, m = 1, \ldots, n,$$

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

$$(3.17) \qquad \sum_{i=1}^{k} p_{(i,m),(i,l)} = \delta_{l,m} - \sum_{\nu=1}^{N} a_{m,l,\nu} \Big(\sum_{i=1}^{k} d_{i,i,\nu} \Big), \quad l, m = 1, \ldots, n.$$

Remark 3.11. Assume that $\mathcal{S}_{\mathbf{A}}$ is an operator system. By Theorem 3.4, if the Interpolation Problem has a solution then there exists a positive semidefinite matrix $\widetilde{D}$ in $D_{\mathbf{A},\mathbf{B}} + M_k \otimes \mathcal{S}_{\mathbf{A}}^{\perp}$ hence, by Lemma 3.3 we have $0 \le \operatorname{tr}(\widetilde{D}) = \operatorname{tr}(D_{\mathbf{A},\mathbf{B}})$. Therefore, under these assumptions, a necessary condition of solvability of the Interpolation Problem is $\operatorname{tr}(D_{\mathbf{A},\mathbf{B}}) \ge 0$.

3.2. **Orthonormalisation of the Input Data.** Theorem 3.4 gives the necessary and sufficient condition of solvability of the Interpolation Problem in terms of the density matrix $D_{\mathbf{A},\mathbf{B}}$ but, in order to precisely get it one might solve the system of linear equations (3.8), with the Gramian matrix $[\operatorname{tr}(A_\mu^* A_\nu)]_{\mu,\nu}$ as the principal matrix of the system. If the matrices $A_1, \ldots, A_N$ 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, the Gram-Schmidt orthonormalisation algorithm yields an orthonormal system of matrices that preserves the assumptions (a1)–(a3), due to the fact that the trace of a product of two Hermitian matrices is always real. More precisely, if $A_1', \ldots, A_N'$ is the Gram-Schmidt orthogonalisation of the sequence of linearly independent Hermitian matrices $A_1, \ldots, A_N$ then

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

$$U_{\nu+1} = A_{\nu+1} - \sum_{\mu=1}^{\nu} \operatorname{tr}(A_\mu' A_\mu) A_\mu, \quad A_{\nu+1}' = \frac{1}{\sqrt{\operatorname{tr}(U_{\nu+1}^2)}} U_{\nu+1}, \quad \nu = 1, \ldots, N-1.$$

Then, we can change, accordingly, the sequence $B_1, \ldots, B_N$ to $B_1', \ldots, B_N'$

$$B_1' = \frac{1}{\sqrt{\operatorname{tr}(A_1^2)}} B_1, \quad B_{\nu+1}' = \frac{1}{\sqrt{\operatorname{tr}(U_{\nu+1}^2)}} \Big(B_{\nu+1} - \sum_{\mu=1}^{\nu} \operatorname{tr}(A_\mu' A_\mu) B_\mu \Big), \quad \nu = 1, \ldots, N-1,$$

and observe that a linear map $\varphi \colon M_n \to M_k$ satisfies the constraints $\varphi(A_\nu) = B_\nu$, $\nu = 1, \ldots, N$, if and only if $\varphi(A_\nu') = B_\nu'$, $\nu = 1, \ldots, N$. Therefore, without loss of generality, we can replace the assumption (a2) with the assumption

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

Lemma 3.12. *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*

$$(3.18) \qquad D_{\mathbf{A},\mathbf{B}} = \sum_{\nu=1}^{N} B_\nu^T \otimes A_\nu.$$

Proof. Under the assumption (a2'), the Gramian matrix of $A_1, \ldots, A_N$ is the identity matrix I_N hence the system of linear equations (3.8) is simply solvable as $d_{i,j,\nu} = \overline{b}_{i,j,\nu} = b_{j,i,\nu}$ for

all $i, j = 1, \ldots, k$ and all $\nu = 1, \ldots, N$, where we have taken into account that B_ν are all Hermitian matrices. Thus, by (3.7), we have

$$D_{\mathbf{A},\mathbf{B}} = \sum_{\nu=1}^{N} \sum_{i,j=1}^{k} b_{j,i,\nu} E_{i,j}^{(k)} \otimes A_\nu = \sum_{\nu=1}^{N} B_\nu^T \otimes A_\nu. \qquad \square$$

Note that under the assumptions (a1) and (a2') we can always find an orthonormal basis $A_1, \ldots, A_N, A_{N+1}, \ldots, A_{n^2}$ of M_n, with respect to the Hilbert-Schmidt inner product, whose first 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 orthonormalisation of a sequence of linearly independent Hermitian matrices.

Theorem 3.13. *Assume that the data $A_1, \ldots, A_N$ and $B_1, \ldots, B_N$ satisfy the assumptions (a1) and (a2'). Let $A_{N+1}, \ldots, A_{n^2}$ be a sequence of Hermitian matrices in M_n such that $A_1, \ldots, A_{n^2}$ is an orthonormal basis of M_n with respect to the Hilbert-Schmidt inner product. The following assertions are equivalent:*

(1) *There exists $\varphi \in \mathrm{CP}(M_n, M_k)$ such that $\varphi(A_\nu) = B_\nu$ for all $\nu = 1, \ldots, N$.*

(2) *There exist numbers $p_{i,j,\nu}$, $i, j = 1, \ldots, k$ and $\nu = N+1, \ldots, n^2$, such that $p_{j,i,\nu} = \overline{p}_{i,j,\nu}$ and*

$$(3.19) \qquad \sum_{\nu=1}^{N} B_\nu^T \otimes A_\nu + \sum_{i,j=1}^{k} \sum_{\nu=N+1}^{n^2} p_{i,j,\nu} E_{i,j}^{(k)} \otimes A_\nu \geq 0.$$

Proof. We use Theorem 3.4, by means of Lemma 3.12 and Lemma 3.3, 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 $D_{\mathbf{A},\mathbf{B}} + P \geq 0$. $\qquad \square$

Remarks 3.14. Assume that the data $A_1, \ldots, A_N$ and $B_1, \ldots, B_N$ satisfy the assumptions (a1) and (a2').

(i) If the set $\mathcal{C}_{\mathbf{A},\mathbf{B}}$ is nonempty, then, as a consequence of Lemma 3.12 and Remark 3.6, the following conditions are necessary:

(a) For arbitrary $\nu = 1, \ldots, N$, if A_ν is semidefinite then B_ν is semidefinite of the same type.

(b) If $\mathcal{S}_{\mathbf{A}}$ is an operator system, then $\sum_{\nu=1}^{N} \mathrm{tr}(B_\nu) \, \mathrm{tr}(A_\nu) \geq 0$.

(ii) On the other hand, from Lemma 3.12 and Remark 3.6.(2), if

$$(3.20) \qquad \sum_{\nu=1}^{N} B_\nu^T \otimes A_\nu \geq 0,$$

then the linear map $\varphi \colon M_n \to M_k$ defined by

$$(3.21) \qquad \varphi(C) = \Big[\sum_{\nu=1}^{N} b_{i,j,\nu}\,\mathrm{tr}(A_\nu C)\Big]_{i,j=1}^{k}, \quad C \in M_n,$$

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

3.3. **A Single Interpolation Pair.** For fixed $n, k \in \mathbb{N}$, consider completely positive maps $\varphi \colon M_n \to M_k$ in the minimal Kraus representation, that is, $\varphi(A) = V^*AV$, for some $V \in M_{k,n}$ and all $A \in M_n$. By Proposition 2.1, this corresponds to the case when the rank of the Choi matrix Φ of φ 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 φ 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 $S_A = \mathrm{sgn}(A)$ is a Hermitian partial isometry, where sgn is the usual sign function: $\mathrm{sgn}(t) = 1$ for $t > 0$, $\mathrm{sgn}(t) = -1$ for $t < 0$, and $\mathrm{sgn}(0) = 0$. Note that, with this notation, $A = S_A|A|$ is the polar decomposition of A. Let $\mathcal{H}_A = \mathbb{C}^n \ominus \mathrm{Null}(A)$ 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 ± 1. Then, with respect to the decomposition

$$(3.22) \qquad \mathbb{C}^n = \mathcal{H}_A^+ \oplus \mathcal{H}_A^- \oplus \mathrm{Null}(A),$$

we have

$$(3.23) \qquad A = \begin{bmatrix} A_+ & 0 & 0 \\ 0 & -A_- & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad S_A = \begin{bmatrix} I_A^+ & 0 & 0 \\ 0 & -I_A^- & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

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* $\kappa_\pm(A) = \dim(\mathcal{H}_A^\pm) = \mathrm{rank}(A_\pm)$ and $\kappa_0(A) = \dim(\mathrm{Null}(A))$. 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

$$(3.24) \qquad [x,y]_A = \langle Ax, y \rangle, \quad x, y \in \mathbb{C}^n.$$

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

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 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 $J_\pm \colon \mathcal{H}_B^\pm \to \mathcal{H}_A^\pm$. In addition to the decomposition (3.22) of $\mathbb{C}^n$ with respect to A, we consider the like decomposition of $\mathbb{C}^k$ with respect to B

$$(3.25) \qquad \mathbb{C}^k = \mathcal{H}_B^+ \oplus \mathcal{H}_B^- \oplus \mathrm{Null}(B),$$

and with respect to it, the block-matrix representation of B similar to (3.23). Then, with respect to (3.22) and (3.25) define $V \in M_{k,n}$ by

$$(3.26) \qquad V = \begin{bmatrix} B_+^{1/2} J_+ A_+^{-1/2} & 0 & 0 \\ 0 & B_-^{1/2} J_- A_-^{-1/2} & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

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

Theorem 3.16. *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 $\varphi \colon M_n \to M_k$ such that $\varphi(A) = B$.*

(ii) *If A is semidefinite, then B is semidefinite of the same type.*

(iii) *There exists $m \in \mathbb{N}$ such that*

$$(3.27) \qquad \kappa_\pm(B) \leq m \, \kappa_\pm(A).$$

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

$$(3.28) \qquad r = \min\{m \in \mathbb{N} \mid \kappa_\pm(B) \leq m \, \kappa_\pm(A)\}.$$

Proof. It takes only a moment of thought to see that the assertions (ii) and (iii) are equivalent. Thus, it remains to prove that the assertions (i) and (iii) are equivalent. Assuming that there exists $m \in \mathbb{N}$ satisfying (3.27), let $r \in \mathbb{N}$ be defined as in (3.28). Then there exist Hermitian matrices $B_1, B_2, \ldots, B_r \in M_k$ such that $\kappa_\pm(B_j) \leq \kappa_\pm(A)$ for all $j = 1, \ldots, r$. By Lemma 3.15 there exist $V_1, V_2, \ldots, V_r \in M_{k,n}$ such that $V_j^* A V_j = B_j$ for all $j = 1, \ldots, r$. Then, letting $\varphi = \sum_{j=1}^r V_j^* \cdot V_j \colon M_n \to M_k$ we obtain a completely positive map such that $\varphi(A) = B$.

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

Note that Theorem 3.16 provides one more (different) argument for Corollary 3.2 in [16], and different from the argument given in Remark 3.6.(3) as well.

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Institute of Mathematics - Romanian Academy, PO Box 1-764, RO 014700 Bucharest, Romania *and* Institute of Mathematics of the Czech Academy, Zitna 25, 11567 Prague 1, Czech Republic

E-mail address: calin.ambrozie@imar.ro

Department of Mathematics, Bilkent University, 06800 Bilkent, Ankara, Turkey, *and* Institutul de Matematică al Academiei Române, C.P. 1-764, 014700 Bucureşti, România

E-mail address: aurelian@fen.bilkent.edu.tr and A.Gheondea@imar.ro