

## Complete positivity of the map from a basis to its dual basis

Vern I. Paulsen<sup>1</sup> and Fred Shultz<sup>2</sup>

<sup>1</sup>*Department of Mathematics, University of Houston, Houston, TX 77204-3476<sup>a</sup>*

<sup>2</sup>*Department of Mathematics, Wellesley College, Wellesley, MA 02481<sup>b</sup>*

The dual of a matrix ordered space has a natural matrix ordering that makes the dual space matrix ordered as well. The purpose of these notes is to give a condition that describes when the linear map taking a basis of  $M_n$  to its dual basis is a complete order isomorphism. We exhibit “natural” orthonormal bases for  $M_n$  such that this map is an order isomorphism, but not a complete order isomorphism. Included among such bases is the Pauli basis. Our results generalize the Choi matrix by giving conditions under which the role of the standard basis  $\{E_{ij}\}$  can be replaced by other bases.

---

<sup>a</sup>Electronic mail: vern@math.uh.edu; The research of the first author was supported by NSF grant 1101231

<sup>b</sup>Electronic mail: fshultz@wellesley.edu

Given a finite dimensional vector space  $V$  there is no “natural” linear isomorphism between  $V$  and the dual space  $V^d$ , but each time we fix a basis  $\mathcal{B} = \{v_i : i \in I\}$  for  $V$  there is a *dual basis*  $\tilde{\mathcal{B}} = \{\delta_i : i \in I\}$  for  $V^d$  satisfying

$$\delta_i(v_j) = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}$$

and this allows us to define a (basis dependent) linear isomorphism between  $V$  and  $V^d$ . We denote by  $L(V)$  the linear maps from  $V$  to  $V$ .

*Definition 1.* Let  $M_n$  denote the vector space of  $n \times n$  complex matrices. If  $\mathcal{B}$  is a basis of  $M_n$ , the linear map from  $M_n$  to  $M_n^d$  taking each member of  $\mathcal{B}$  to the corresponding member of the dual basis is denoted by  $\mathcal{D}_{\mathcal{B}}$ , and is called the *duality map*. We let  $\Gamma_{\mathcal{B}} = \mathcal{D}_{\mathcal{B}}^{-1} : M_n^d \rightarrow M_n$  denote the inverse of this map.

Note that if  $f \in M_n^d$ , and  $\mathcal{B}$  is a basis of  $M_n$ , then  $\Gamma_{\mathcal{B}}(f) = \sum_{b \in \mathcal{B}} f(b)b$ . In particular, when we let  $\mathcal{E} = \{E_{ij} : 1 \leq i, j \leq n\}$  denote the standard matrix units, then the map  $\Gamma_{\mathcal{E}} : M_n^d \rightarrow M_n$  satisfies

$$\Gamma_{\mathcal{E}}(f) = \sum_{i,j=1}^n f(E_{ij})E_{ij}.$$

*Definition 2.* If  $f \in M_n^d$ , there is a unique matrix  $D$  such that  $f(X) = \text{tr}(DX)$  for all  $X \in M_n$ , and we call this matrix the *density matrix* for  $f$ , with no requirement of positivity for  $f$  or  $D$ .

We denote the transpose map by  $t : M_n \rightarrow M_n$ , and for  $D \in M_n$  we write  $D^t$  instead of  $t(D)$ . We have

$$f(X) = \text{tr}(\Gamma_{\mathcal{E}}(f)^t X) \text{ for all } X \in M_n. \quad (1)$$

Thus  $\Gamma_{\mathcal{E}}$  is just the map that identifies a functional  $f$  with the transpose of its density matrix.

This note is motivated by the following result of Paulsen-Todorov-Tomforde in Theorem 6.2 of Ref. ? , which we will see later is a restatement of the Choi-Jamiolkowski correspondences? ? .

**Theorem 3.** *The map  $\mathcal{D}_{\mathcal{E}} : M_n \rightarrow M_n^d$  is a complete order isomorphism between these matrix ordered spaces.*

In this paper, we will show that this theorem is very dependent on the choice of basis. In fact, we will show that there exist orthonormal bases for  $M_n$  such that the inverse duality map does not even send positive functionals to positive matrices. Even more intriguing, we will show that there are “natural” orthonormal bases for  $M_n$  such that the inverse duality map does send positive functionals to positive matrices, yet does not associate completely positive maps with positive block matrices. These results can be interpreted as giving some new Choi-Jamiołkowski type results.

We believe that such bases might be useful as entanglement witnesses. (We will comment further on this after Corollary ??).

Before proceeding it will be necessary to establish some notation. The complex conjugate of a complex number  $z$  is denoted by  $\bar{z}$ , and the conjugate transpose of a matrix  $D$  is denoted  $D^*$ . If  $D = (d_{ij})$  is any matrix, then we define  $\bar{D} = (\bar{d}_{ij})$ . Inner products are linear in the first factor unless specified otherwise.

Recall that when we say that a vector space  $V$  is *matrix ordered* we mean that for each natural number  $p$ , we have specified a cone  $C_p$  in the vector space of  $p \times p$  matrices over  $V$ ,  $M_p(V)$ , which we identify as the *positive elements* in  $M_p(V)$ , and that these cones must satisfy certain natural axioms, such as if  $A \in C_p$  and  $B \in C_q$ , then  $A \oplus B \in C_{p+q}$ . We also require that if  $X = (x_{ij})$  is a  $p \times q$  matrix of scalars and  $A = (v_{ij}) \in C_p$ , then

$$X^*AX = \left( \sum_{k,l=1}^p \bar{x}_{ki}v_{kl}x_{lj} \right) \in C_q.$$

When there is no ambiguity we simply write  $C_p = M_p(V)^+$ . See Chapter 13 of Ref. ? for more background on matrix ordered spaces.

Matrix ordered spaces are the natural setting for studying *completely positive maps*. Indeed, given matrix ordered spaces  $V, W$  we say that a linear map  $\Phi : V \rightarrow W$  is completely positive provided that for each  $p$ ,  $(v_{ij}) \in M_p(V)^+$  implies that  $(\Phi(v_{ij})) \in M_p(W)^+$ . (We will denote the map that takes  $(v_{ij})$  to  $(\Phi(v_{ij}))$  by  $\Phi^{(p)}$ , so that  $\Phi$  is completely positive iff every map  $\Phi^{(p)}$  is a positive map.) We say that  $\Phi$  is a complete order isomorphism provided that  $\Phi$  is invertible and that  $\Phi$  and  $\Phi^{-1}$  are both completely positive.

The most frequently encountered example of a matrix ordered space is  $L(H)$ , the bounded linear operators on a Hilbert space  $H$ . We define the matrix ordering by identifying  $M_p(L(H)) = L(H \oplus \cdots \oplus H)$ , the bounded linear operators on the direct sum of  $p$  copies of the Hilbert space, and declaring  $(A_{ij}) \in M_p(L(H))^+$  exactly when it defines a

positive operator on the Hilbert space  $H \oplus \dots \oplus H$ . More broadly, matrix ordered spaces include *operator systems*: norm closed subspaces of  $L(H)$ , which are self-adjoint (i.e. are closed under the map  $A \mapsto A^*$ ) and unital (i.e., contain the identity). Indeed, operator systems can be characterized as matrix ordered spaces satisfying an additional axiom asserting the existence of an element that in an order-theoretic sense acts like the identity in  $L(H)$ , see Ref. ? .

When  $H = \mathbb{C}^n$ , the standard  $n$ -dimensional Hilbert space, we write  $e_1, \dots, e_n$  for the standard basis of  $\mathbb{C}^n$ , and write  $\langle \cdot, \cdot \rangle$  for the inner product on  $\mathbb{C}^n$ . We identify  $L(\mathbb{C}^n)$  with  $M_n$ , the set of  $n \times n$  matrices with entries in  $\mathbb{C}$ . Note that identifying  $M_p(M_n)$ , the  $p \times p$  block matrices with entries from  $M_n$ , with  $M_{pn}$  yields the same cone of positive matrices as when we identify  $M_p(M_n)$  with the linear maps on the direct sum of  $p$  copies of  $\mathbb{C}^n$ ,  $L(\mathbb{C}^n \oplus \dots \oplus \mathbb{C}^n)$ .

Finally, given a matrix ordered space  $V$  there is a natural way to define a matrix ordering on the dual space  $V^d$ . To do this we declare that a matrix of functionals  $(f_{ij}) \in M_p(V^d)$  belongs to  $M_p(V^d)^+$  if and only if the linear map  $\Phi : V \rightarrow M_p$  given by  $\Phi(v) = (f_{ij}(v))$  is completely positive.

In this paper we will be concerned with examining various natural bases  $\mathcal{B}$  for  $M_n$  and determining whether or not the duality map  $\mathcal{D}_{\mathcal{B}}$  is a complete order isomorphism. We will see that there exist bases for  $M_n$  such that  $\mathcal{D}_{\mathcal{B}}$  is positive but not completely positive.

Since our results rely on Theorem ??, we present a new proof here, that is somewhat simpler than the proof that appeared in Ref. ? .

*Proof of Theorem ??.* Rather than proving that  $\mathcal{D}_{\mathcal{E}}$  is a complete order isomorphism, we prove, equivalently, that  $\Gamma_{\mathcal{E}} = \mathcal{D}_{\mathcal{E}}^{-1} : M_n^d \rightarrow M_n$  is a complete order isomorphism. We have already seen that  $\Gamma_{\mathcal{E}}$  sends functionals to the transpose of their density matrices. Since a functional is positive if and only if its density matrix is positive, and the transpose map is an order isomorphism, we see that  $\Gamma_{\mathcal{E}}$  is an order isomorphism.

Now let  $(f_{k,l}) \in M_p(M_n^d)$  and consider the map  $\Phi : M_n \rightarrow M_p$  defined by  $\Phi(X) = (f_{k,l}(X)) = \sum_{k,l=1}^p f_{k,l}(X)E_{k,l}$ . We must show that  $\Phi$  is completely positive if and only if  $\Gamma_{\mathcal{E}}^{(p)}((f_{k,l})) \in M_p(M_n)^+$ .

We have

$$\Gamma_{\mathcal{E}}^{(p)}((f_{k,l})) = (\Gamma_{\mathcal{E}}(f_{k,l}))_{k,l=1}^p = \left( \sum_{i,j=1}^n f_{k,l}(E_{ij})E_{ij} \right)_{k,l=1}^p$$

$$\begin{aligned}
&= \sum_{k,l=1}^p E_{k,l} \otimes \left[ \sum_{i,j=1}^n f_{k,l}(E_{ij}) E_{ij} \right] \\
&= \sum_{i,j=1}^n \left[ \sum_{k,l=1}^p f_{k,l}(E_{ij}) E_{k,l} \right] \otimes E_{ij} \\
&= \sum_{i,j=1}^n \Phi(E_{ij}) \otimes E_{ij}.
\end{aligned}$$

Since the map that takes  $A \otimes B$  to  $B \otimes A$  extends to a \*-isomorphism of  $M_p \otimes M_n$  onto  $M_n \otimes M_p$ , the last expression is positive iff the matrix

$$C_\Phi = \sum_{i,j=1}^n E_{ij} \otimes \Phi(E_{ij}) \quad (2)$$

is positive. But this last matrix is the Choi matrix and by Choi's theorem<sup>?</sup> the map  $\Phi$  is completely positive if and only if this block matrix is positive. Thus  $(f_{k,l}) \in M_p(M_n)^+$  if and only if  $(\Gamma_{\mathcal{E}}(f_{k,l})) \in M_p(M_n)^+$  and we have shown that  $\Gamma_{\mathcal{E}}$  is a complete order isomorphism. This completes the proof of Theorem ?? □

A map  $\Psi : M_n \rightarrow M_n$  or  $\Psi : M_n^d \rightarrow M_n$  is called a *co-positive order isomorphism* provided that its composition  $t \circ \Psi$  with the transpose map  $t$  on  $M_n$  is a complete order isomorphism.

**Corollary 4.** *The linear map from  $M_n^d$  to  $M_n$  that takes a functional to its density matrix is a co-positive order isomorphism.*

*Proof.* As remarked in connection with equation (??), the map that takes a functional to its density matrix is  $t \circ \Gamma_{\mathcal{E}}$ . □

Now that we have a complete order isomorphism  $\mathcal{D}_{\mathcal{E}}$  between  $M_n$  and  $M_n^d$ , in order to determine whether or not other maps between  $M_n$  and  $M_n^d$  are complete order isomorphisms, it will be convenient to work with a map  $\tilde{\mathcal{D}}_{\mathcal{B}} : M_n \rightarrow M_n$  instead of  $\mathcal{D}_{\mathcal{B}} : M_n \rightarrow M_n^d$ .

*Definition 5.* Let  $\mathcal{B}$  be a basis of  $M_n$  and  $\mathcal{E}$  the standard basis of matrix units. Then we define  $\tilde{\mathcal{D}}_{\mathcal{B}} : M_n \rightarrow M_n$  by  $\tilde{\mathcal{D}}_{\mathcal{B}} = \Gamma_{\mathcal{E}} \circ \mathcal{D}_{\mathcal{B}}$ .

Note that since  $\Gamma_{\mathcal{E}}$  is a complete order isomorphism,  $\mathcal{D}_{\mathcal{B}}$  will be a complete order isomorphism if and only if  $\tilde{\mathcal{D}}_{\mathcal{B}}$  is a complete order isomorphism.

Recall that  $\mathcal{E} = \{E_{ij}\}$  is an orthonormal basis for  $M_n$  with respect to the Hilbert-Schmidt inner product, which we denote by  $\langle A, B \rangle = \text{tr}(AB^*)$ , where  $\text{tr} : M_n \rightarrow \mathbb{C}$  denotes

the unnormalized trace,  $\text{tr}(A) = \sum_{i=1}^n a_{ii}$ . We fix an order for the basis  $\mathcal{E}$ , and represent elements in  $L(M_n)$  as  $n^2 \times n^2$  matrices. Given  $L \in L(M_n)$  we write  $[L]$  for the matrix for  $L$  with respect to the basis  $\mathcal{E}$ . For an  $n^2 \times n^2$  matrix  $M$ , we denote its transpose by  $M^T$ , to distinguish this transpose from the transpose  $t$  on  $M_n$ , and  $M^*$  denotes the conjugate transpose. If  $L \in L(M_n)$ , then  $L^*$  denotes the adjoint with respect to the Hilbert-Schmidt inner product, i.e.,  $\langle L^*(A), B \rangle = \langle A, L(B) \rangle$  for all  $A, B \in M_n$ , and we have  $[L]^* = [L^*]$ .

*Definition 6.* Let  $\mathcal{B}$  be a basis of  $M_n$  and  $\mathcal{E}$  the standard basis of matrix units. A *change of basis map* is any linear map  $C_{\mathcal{B}}$  in  $L(M_n)$  taking the set  $\mathcal{E}$  to the set  $\mathcal{B}$ . By slight abuse of notation, we write  $C_{\mathcal{B}}^T$  for the unique linear map in  $L(M_n)$  whose matrix in the standard basis  $\mathcal{E}$  is the transpose of the matrix of  $C_{\mathcal{B}}$ , so that  $[C_{\mathcal{B}}^T] = [C_{\mathcal{B}}]^T$ . We define  $M_{\mathcal{B}} = C_{\mathcal{B}}C_{\mathcal{B}}^T \in L(M_n)$ .

Since a linear map is uniquely determined by its values on a basis, we see that a change of basis map is uniquely determined up to re-orderings of the basis elements. Thus, in the setting of  $M_n$  there will be  $(n^2)!$  change of basis maps. However, the map  $M_{\mathcal{B}}$  is independent of the choice of change of basis map or matrix. Indeed, fix one change of basis map  $C_{\mathcal{B}}$ . Then every change of basis map has the form  $C_{\mathcal{B}} \circ P$ , where  $P \in M_n$  is a linear map which permutes the basis  $\mathcal{E}$ . Since  $P$  sends the orthonormal basis  $\mathcal{E}$  to itself, its matrix in that basis is orthogonal. Thus  $M_{\mathcal{B}}$  is unchanged if we replace  $C_{\mathcal{B}}$  by  $C_{\mathcal{B}}P$ .

Fortunately, we will find that the results that we seek depend on  $M_{\mathcal{B}}$  and are independent of the choice of change of basis map  $C_{\mathcal{B}}$ . In particular, our conditions determining when the duality map  $\mathcal{D}_{\mathcal{B}}$  is an order isomorphism or a complete order isomorphism will be expressed in terms of the map  $M_{\mathcal{B}}$ .

**Theorem 7.** *If  $\mathcal{B}$  is a basis of  $M_n$ , then the duality map is given by  $\mathcal{D}_{\mathcal{B}} = \mathcal{D}_{\mathcal{E}} \circ M_{\mathcal{B}}^{-1}$ .*

*Proof.* Let  $\mathcal{B} = \{X_1, \dots, X_{n^2}\}$ , and let  $\{\widehat{X}_1, \dots, \widehat{X}_{n^2}\} \subset M_n^d$  be the dual basis. Using the fixed order for  $\mathcal{E}$ , we write  $\mathcal{E} = \{E_1, \dots, E_{n^2}\}$ .

Define  $Y_j = \mathcal{D}_{\mathcal{E}}^{-1}(\widehat{X}_j) = \Gamma_{\mathcal{E}}(\widehat{X}_j) \in M_n$ . We are going to show

$$C_{\mathcal{B}}^T Y_j = E_j \text{ for all } j. \quad (3)$$

Recall that  $\overline{Y}_j \in M_n$  is the matrix whose entries are the complex conjugates of those of  $Y_j$ .

For each  $i, j$ , using (??)

$$\begin{aligned}
\langle E_i, C_{\mathcal{B}}^* \overline{Y_j} \rangle &= \langle C_{\mathcal{B}} E_i, \overline{Y_j} \rangle = \langle X_i, \overline{Y_j} \rangle = \text{tr}(X_i \overline{Y_j}^*) \\
&= \text{tr}(X_i Y_j^t) = \text{tr}(X_i (\Gamma_{\mathcal{E}}(\widehat{X}_j))^t) \\
&= \widehat{X}_j(X_i) = \delta_{ij}.
\end{aligned} \tag{4}$$

It follows that  $C_{\mathcal{B}}^* \overline{Y_j} = E_j$ .

For  $Y \in M_n$  let  $[Y] \in \mathbb{C}^{n^2}$  denote the coordinate vector for  $Y$  with respect to the basis  $\mathcal{E}$ , viewed as a column matrix. Then

$$e_j = [E_j] = [C_{\mathcal{B}}^* \overline{Y_j}] = [C_{\mathcal{B}}^*][\overline{Y_j}] = [C_{\mathcal{B}}]^*[\overline{Y_j}].$$

Conjugating both sides of  $[E_j] = [C_{\mathcal{B}}]^*[\overline{Y_j}]$  gives

$$[E_j] = [C_{\mathcal{B}}]^T[Y_j] = [C_{\mathcal{B}}^T][Y_j] = [\widehat{C}_{\mathcal{B}}^T Y_j],$$

proving (??).

Now

$$C_{\mathcal{B}} C_{\mathcal{B}}^T \mathcal{D}_{\mathcal{E}}^{-1} \widehat{X}_j = C_{\mathcal{B}} C_{\mathcal{B}}^T Y_j = C_{\mathcal{B}} E_j = X_j = \mathcal{D}_{\mathcal{B}}^{-1} \widehat{X}_j,$$

so by linearity  $M_{\mathcal{B}} \mathcal{D}_{\mathcal{E}}^{-1} = \mathcal{D}_{\mathcal{B}}^{-1}$ . Thus  $\mathcal{D}_{\mathcal{B}} = \mathcal{D}_{\mathcal{E}} M_{\mathcal{B}}^{-1}$ . □

*Notation.* If  $C \in M_n$ , then  $\Phi_C : M_n \rightarrow M_n$  is the completely positive map defined by  $\Phi_C(X) = CXC^*$ .

Recall that a map  $\Psi : M_n \rightarrow M_p$  is called *completely co-positive* if and only if  $t \circ \Psi$  is completely positive, and a map  $\Psi : M_n \rightarrow M_n$  is called a *co-positive order isomorphism* provided that its composition  $t \circ \Psi$  with the transpose map  $t$  on  $M_n$  is a complete order isomorphism. Here the order of composition with the transpose map doesn't matter as shown by the next result.

**Proposition 8.** *Let  $\Phi : M_n \rightarrow M_p$  then  $t \circ \Phi$  is completely positive if and only if  $\Phi \circ t$  is completely positive.*

*Proof.* By Choi's result<sup>?</sup>,  $t \circ \Phi$  is completely positive if and only if  $(\Phi(E_{ij})^t)$  is positive, while  $\Phi \circ t$  is completely positive if and only if  $(\Phi(E_{j,i}))$  is positive. But these  $np \times np$  matrices are transposes of each other. □

We start with the following description of order automorphisms of  $M_n$  and their partition into completely positive and completely co-positive maps. It is a consequence of more general results of Kadison<sup>?</sup> relating isometries, Jordan isomorphisms, order isomorphisms, and \*-isomorphisms of C\*-algebras, specialized to  $M_n$  viewed as a C\*-algebra.

**Lemma 9.** *Let  $\Phi : M_n \rightarrow M_n$  be an order isomorphism. Then there exists an invertible  $C \in M_n$  such that either  $\Phi = \Phi_C$  or  $\Phi = t \circ \Phi_C$ . In the first case,  $\Phi$  is a complete order isomorphism, and in the second case  $\Phi$  is a co-positive order isomorphism. If  $n > 1$ , both cases cannot occur simultaneously.*

*Proof.* First assume  $\Phi$  is unital, i.e., that  $\Phi(I) = I$ . For Hermitian matrices  $A$ , we have  $\|A\| = \sup\{\lambda \in \mathbb{R} \mid -\lambda I \leq A \leq \lambda I\}$ , so a unital order isomorphism is an isometry on Hermitian elements of  $M_n$ . It follows that  $\Phi$  is an isometry on all of  $M_n$ , cf. proof of Theorem 5 in Ref. ? . Every unital isometry on  $M_n$  is a Jordan isomorphism, i.e., preserves the Jordan product  $A \circ B = (1/2)(AB + BA)$ , cf. Theorem 7 of Ref. ? . Every Jordan isomorphism on  $M_n$  is a \*-isomorphism or \*-anti-isomorphism, cf. Corollary 11 of Ref. ? . In the latter case, composing with the transpose map gives a \*-isomorphism. It is well known that every \*-isomorphism of  $M_n$  is conjugation by a unitary, see, for example, Theorem 4.27 of Ref. ? . Thus there is a unitary  $U$  such that  $\Phi = \Phi_U$  or  $\Phi = t \circ \Phi_U$ .

Finally, let  $\Phi$  be an arbitrary order isomorphism. We will show  $\Phi(I)$  is invertible. Observe that  $0 \leq A \in M_n$  is invertible iff  $A$  is an order unit, i.e., if for all  $B = B^* \in M_n$  there exists  $\lambda \in \mathbb{R}$  such that  $-\lambda A \leq B \leq \lambda A$ . An order isomorphism takes order units to order units, so  $\Phi(1)$  is invertible. Let  $D = \Phi(1)^{1/2}$ , and define  $\Psi = \Phi_{D^{-1}} \circ \Phi$ . Then  $\Psi$  is a unital order isomorphism, so by the first paragraph there exists a unitary  $U$  such that  $\Psi = \Phi_U$  or  $\Psi = t \circ \Phi_U$ . Then  $\Phi = \Phi_D \circ \Psi = \Phi_D \circ \Phi_U = \Phi_{DU}$ , or else  $\Phi = \Phi_D \circ t \circ \Phi_U = t \circ \Phi_C$  where  $C = D^t U$ . Note that if both cases occur then  $\Psi$  is both a \*-isomorphism and a \*-anti-isomorphism, which is possible only if  $M_n$  is abelian, and that holds only when  $n = 1$ .  $\square$

Note that Lemma ?? implies that a composition of two complete order isomorphisms, or two co-positive order isomorphisms, is a complete order isomorphism, and a composition of a complete order isomorphism and a co-positive order isomorphism (in either order) is a co-positive order isomorphism.



**Theorem 10.** *Let  $\mathcal{B}$  be a basis of  $M_n$ . Then  $\mathcal{D}_{\mathcal{B}}$  is an order isomorphism iff there exists  $C \in M_n$  such that either (1)  $M_{\mathcal{B}} = \Phi_C$  or (2)  $M_{\mathcal{B}} = t \circ \Phi_C$ . In the first case,  $\mathcal{D}_{\mathcal{B}}$  is a complete order isomorphism, and in the second case it is a co-positive order isomorphism.*

*Proof.* By Theorem ??, we have  $\mathcal{D}_{\mathcal{B}} = \mathcal{D}_{\mathcal{E}} \circ M_{\mathcal{B}}^{-1}$ . Since  $\mathcal{D}_{\mathcal{E}}$  is a complete order isomorphism (Theorem ??), then  $\mathcal{D}_{\mathcal{B}}$  is a complete order isomorphism (respectively, co-positive order isomorphism) if and only if  $M_{\mathcal{B}}$  is a complete order isomorphism (respectively, co-positive order isomorphism). Now the theorem follows from Lemma ??.  $\square$

**Corollary 11.** *Let  $\mathcal{B} = \{B_j : 1 \leq j \leq n^2\}$  be a basis for  $M_n$ .*

1.  $M_{\mathcal{B}} = \Phi_C$  for some  $C \in M_n$  if and only if  $\Gamma_{\mathcal{B}} : M_n^d \rightarrow M_n$  is a complete order isomorphism,
2.  $M_{\mathcal{B}} = t \circ \Phi_C$  for some  $C \in M_n$  if and only if  $t \circ \Gamma_{\mathcal{B}} : M_n^d \rightarrow M_n$  is a complete order isomorphism.

*Proof.* We prove the second statement. By Theorem ??,  $M_{\mathcal{B}} = t \circ \Phi_C$  iff  $\mathcal{D}_{\mathcal{B}}$  is a co-positive order isomorphism. This is equivalent to  $\Gamma_{\mathcal{B}} = \mathcal{D}_{\mathcal{B}}^{-1}$  being a co-positive order isomorphism, and hence to  $t \circ \Gamma_{\mathcal{B}}$  being a complete order isomorphism.  $\square$

Both Choi and Jamiołkowski have defined useful correspondences that associate a matrix in  $M_n \otimes M_p$  with each linear map  $\Phi : M_n \rightarrow M_p$ . Choi's correspondence is  $\Phi \mapsto C_{\Phi}$ , where

$$C_{\Phi} = \sum_{ij} E_{ij} \otimes \Phi(E_{ij}). \quad (5)$$

As remarked in the proof of Theorem ??, positivity of the Choi matrix (??) is equivalent to positivity of  $\sum_{ij} \Phi(E_{ij}) \otimes E_{ij}$ , and it is this latter form that we generalize below. We now describe a related correspondence defined by Jamiołkowski<sup>?</sup>. If  $\Phi : M_n \rightarrow M_p$ , then  $\mathcal{J}(\Phi)$  is defined by the condition  $\langle \mathcal{J}(\Phi), A^* \otimes B \rangle = \langle \Phi(A), B \rangle$  for all  $A \in M_n$ ,  $B \in M_p$ . This is equivalent to

$$\mathcal{J}(\Phi) = \sum_{ij} E_{ij}^* \otimes \Phi(E_{ij}). \quad (6)$$

Regarding our current investigation, the Choi matrix  $C_{\Phi}$  has the property that  $C_{\Phi} \geq 0$  iff  $\Phi$  is completely positive<sup>?</sup>. The Jamiołkowski correspondence has the property that in (??),  $\mathcal{J}(\Phi)$  is unchanged if the basis  $\{E_{ij}\}$  is replaced by any orthonormal basis of  $M_n$ . Our correspondence will be closer to Choi's.

**Corollary 12.** *Let  $\mathcal{B} = \{B_j : 1 \leq j \leq n^2\}$  be a basis for  $M_n$ , and let  $\Psi : M_n \rightarrow M_p$  be a linear map.*

1. *If  $M_{\mathcal{B}} = \Phi_C$  for some  $C \in M_n$ , then  $\Psi$  is completely positive if and only if  $\sum_{j=1}^{n^2} \Psi(B_j) \otimes B_j \in (M_p \otimes M_n)^+$ .*
2. *If  $M_{\mathcal{B}} = t \circ \Phi_C$  for some  $C \in M_n$ , then  $\Psi$  is completely positive if and only if  $\sum_{j=1}^{n^2} \Psi(B_j) \otimes B_j^t \in (M_p \otimes M_n)^+$ .*
3. *If  $M_{\mathcal{B}} = t \circ \Phi_C$  for some  $C \in M_n$ , then  $\Psi$  is completely co-positive if and only if  $\sum_{j=1}^{n^2} \Psi(B_j) \otimes B_j \in (M_p \otimes M_n)^+$ .*

*Proof.* To prove the first statement, for  $1 \leq k, l \leq p$  define  $f_{k,l} \in M_n^d$  by  $\Psi(X) = (f_{k,l}(X))$ . Then by the definition of the order on  $M_p(M_n^d)$  discussed earlier,  $\Psi$  is completely positive if and only if  $(f_{k,l}) \in M_p(M_n^d)^+$  which holds if and only if  $(\Gamma_{\mathcal{B}}(f_{k,l})) \in M_p(M_n)^+$ , cf. Theorem ???. But as in the proof of Theorem ??, we have that

$$(\Gamma_{\mathcal{B}}(f_{k,l})) = \sum_{j=1}^{n^2} \Psi(B_j) \otimes B_j.$$

To prove the second statement, note that  $\Psi$  is completely positive if and only if  $(t \circ \Gamma_{\mathcal{B}}(f_{k,l})) \in M_p(M_n)^+$  and this matrix is seen to be equal to

$$\sum_{j=1}^{n^2} \Psi(B_j) \otimes B_j^t.$$

For the third statement, replace  $\Psi$  by  $t \circ \Psi$  in the second statement. This shows  $\Psi$  is completely co-positive iff  $\sum_{j=1}^{n^2} \Psi(B_j)^t \otimes B_j^t \in (M_p \otimes M_n)^+$ , and now applying the transpose map gives (3).  $\square$

We now point out that bases with the properties indicated in the Corollary are related to entanglement witnesses. Indeed suppose  $\mathcal{B} = \{B_1, \dots, B_{n^2}\}$  is a basis of  $M_n$  for which Corollary ??? (1) holds. Taking  $\Phi = I$  we have  $\sum_i B_i \otimes B_i \geq 0$ . Let  $\Phi : M_n \rightarrow M_n$  be a map that is positive but not completely positive. Define

$$B_0 = \sum_i B_i \otimes B_i \text{ and } B_{\Phi} = \sum_i \Phi(B_i) \otimes B_i.$$

Then for any positive  $X, Y$ , since  $\Phi \geq 0$ , we have

$$\begin{aligned} \langle B_\Phi, X \otimes Y \rangle &= \left\langle \sum_i \Phi(B_i) \otimes B_i, X \otimes Y \right\rangle \\ &= \langle (\Phi \otimes I)B_0, X \otimes Y \rangle \\ &= \langle B_0, \Phi^*(X) \otimes Y \rangle \geq 0, \end{aligned} \tag{7}$$

and hence  $B_\Phi$  is  $\geq 0$  on all separable states. Since  $\Phi$  is not completely positive, then  $B_\Phi \not\geq 0$ , so there is a state  $A$  such that  $\langle B_\Phi, A \rangle \not\geq 0$ . Such a state is then entangled, so  $B_\Phi$  is an entanglement witness.

## EXAMPLES

*Notation.* If  $x, y \in \mathbb{C}^n$ , then  $R_{x,y} \in M_n$  is the rank one operator defined by  $R_{x,y}z = \langle z, y \rangle x$ . Observe that  $E_{ij} = R_{e_i, e_j}$ .

**Proposition 13.** *Let  $(\lambda_{ij}) \in M_n$ , with all  $\lambda_{ij}$  nonzero, and let  $\mathcal{B}$  be the basis  $\{\lambda_{ij}E_{ij}\}$ . Then  $\mathcal{D}_\mathcal{B}$  is an order isomorphism if and only if the matrix  $(\lambda_{ij}^2)$  is positive semi-definite with rank one. In that case, there are scalars  $\alpha_1, \dots, \alpha_n$  such that  $\lambda_{ij}^2 = \alpha_i \bar{\alpha}_j$ , and if  $C = \text{diag}(\alpha_1, \dots, \alpha_n)$ , then  $\tilde{\mathcal{D}}_\mathcal{B} = \Phi_C$ , and hence  $\mathcal{D}_\mathcal{B}$  is a complete order isomorphism.*

*Proof.* Note that for  $\mathcal{B}$  as described in the proposition, the matrix for  $C_\mathcal{B}$  is diagonal for the standard basis  $\mathcal{E}$  of  $M_n$ , so  $C_\mathcal{B}^T = C_\mathcal{B}$ . Thus  $M_\mathcal{B}(E_{ij}) = (C_\mathcal{B}C_\mathcal{B}^T)(E_{ij}) = \lambda_{ij}^2 E_{ij}$ .

Suppose that the map  $\tilde{\mathcal{D}}_\mathcal{B} : M_n \rightarrow M_n$  is an order isomorphism. We first consider the case where  $\tilde{\mathcal{D}}_\mathcal{B}^{-1} = M_\mathcal{B} = \Phi_C$ . Then  $\Phi_C(E_{ij}) = \lambda_{ij}^2 E_{ij}$ , so

$$\lambda_{ij}^2 E_{ij} = CE_{ij}C^* = CR_{e_i, e_j}C^* = R_{Ce_i, Ce_j}.$$

The ranges of the two sides must coincide, so for each  $i$  there is a scalar  $\alpha_i$  such that  $Ce_i = \alpha_i e_i$ . Substituting into the displayed equation gives  $\lambda_{ij}^2 E_{ij} = \alpha_i \bar{\alpha}_j E_{ij}$ , so  $\lambda_{ij}^2 = \alpha_i \bar{\alpha}_j$ . Thus the matrix  $(\lambda_{ij}^2)$  has rank one and is positive. Conversely, if  $(\lambda_{ij}^2)$  is positive with rank one, then there are nonzero scalars  $\alpha_1, \dots, \alpha_n$  such that  $\alpha_i \bar{\alpha}_j = \lambda_{ij}^2$ . If  $C = \text{diag}(\alpha_1, \dots, \alpha_n)$ , then one readily verifies that  $M_\mathcal{B} = \Phi_C$ . Then  $\tilde{\mathcal{D}}_\mathcal{B}^{-1}$  is a complete order isomorphism, and hence so is  $\mathcal{D}_\mathcal{B}$ .

Now we examine the possibility that  $C_\mathcal{B}C_\mathcal{B}^T = t \circ \Phi_C$ . Then

$$\lambda_{ij}^2 E_{ij} = (CE_{ij}C^*)^t = C^{*t} E_{ji} C^t.$$

Let  $D = C^{*t}$ , so that  $\lambda_{ij}^2 E_{ij} = DE_{ji}D^*$ . Then for all  $i, j$

$$\lambda_{ij}^2 R_{e_i, e_j} = R_{De_j, De_i}.$$

This implies that  $De_j$  is a multiple of  $e_i$  for all  $i, j$ , which is impossible.  $\square$

*Example 14.* If  $C \in M_n$  is invertible, then  $\Phi_C^T = \Phi_{C^t}$ , so  $\Phi_C \Phi_C^T = \Phi_{CC^t}$ . Hence for the basis  $\mathcal{B} = \{\Phi_C(E_{ij})\}$ , we have  $M_{\mathcal{B}} = \Phi_{CC^t}$ , so by Theorem ??,  $\mathcal{B}$  has the property that the map from this basis to its dual basis is a complete order isomorphism. In particular, if  $\{F_{ij}\}$  is any system of matrix units for  $M_n$ , there is a unitary  $V$  such that  $\Phi_V$  satisfies  $\Phi_V(E_{ij}) = F_{ij}$  for all  $i, j$ , and so the map from  $\{F_{ij}\}$  to its dual basis is a complete order isomorphism.

On the other hand, if  $U : M_n \rightarrow M_n$  is unitary with respect to the Hilbert Schmidt inner product and takes  $\mathcal{E}$  to a basis  $\mathcal{B}$ , it need not be the case that the duality map  $\mathcal{D}_{\mathcal{B}}$  is a complete order isomorphism, as can be seen from Proposition ?? with  $\lambda_{11} = i$  and  $\lambda_{ij} = 1$  for  $(i, j) \neq (1, 1)$ . Hence, not every orthonormal basis of  $M_n$  has the property that the duality map is an order isomorphism.

For our next application we study the Pauli spin matrices.

**Theorem 15.** *Let  $\mathcal{B} = \{\sigma_0, \sigma_1, \sigma_2, \sigma_3\}$  be the Pauli spin matrices, i.e.,*

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

*Then the duality map  $\mathcal{D}_{\mathcal{B}}$  is a co-positive order isomorphism. Furthermore, let  $\Psi : M_{2^n} \rightarrow M_p$  be a linear map. Then  $\Psi$  is completely positive if and only if*

$$\sum_{i_1, \dots, i_n=0}^3 \Psi(\sigma_{i_1} \otimes \dots \otimes \sigma_{i_n}) \otimes \sigma_{i_1}^t \otimes \dots \otimes \sigma_{i_n}^t$$

*is a positive  $2^n p \times 2^n p$  matrix.*

*Similarly,  $\Psi$  is completely co-positive if and only if*

$$\sum_{i_1, \dots, i_n=0}^3 \Psi(\sigma_{i_1} \otimes \dots \otimes \sigma_{i_n}) \otimes \sigma_{i_1} \otimes \dots \otimes \sigma_{i_n}$$

*is a positive  $2^n p \times 2^n p$  matrix.*

*Proof.* Let  $C_{\mathcal{B}}$  be the linear map such that

$$C_{\mathcal{B}}(E_{11}) = \sigma_0, \quad C_{\mathcal{B}}(E_{12}) = \sigma_1, \quad C_{\mathcal{B}}(E_{21}) = \sigma_2, \quad C_{\mathcal{B}}(E_{22}) = \sigma_3.$$

Then the matrix for  $M_{\mathcal{B}} = C_{\mathcal{B}}C_{\mathcal{B}}^T$  in the standard basis of  $M_2$  is

$$[C_{\mathcal{B}}][C_{\mathcal{B}}^T] = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

which is twice the matrix of the transpose map  $t : M_2 \rightarrow M_2$ . Thus  $\mathcal{D}_{\mathcal{B}}$  in this case is a co-positive order isomorphism.

Applying Corollary ??, we see that a map  $\Psi : M_2 \rightarrow M_p$  is completely positive if and only if

$$\sum_{j=0}^3 \Psi(\sigma_j) \otimes \sigma_j^t \in (M_p \otimes M_2)^+.$$

Using the explicit form of the Pauli matrices, we obtain that  $\Psi$  is completely positive if and only if

$$\begin{bmatrix} \Psi(\sigma_0) + \Psi(\sigma_3), & \Psi(\sigma_1) + i\Psi(\sigma_2) \\ \Psi(\sigma_1) - i\Psi(\sigma_2), & \Psi(\sigma_0) - \Psi(\sigma_3) \end{bmatrix}$$

is positive in  $M_2(M_p)$ , which is identical to Choi's theorem.

On  $M_{2^n}$  the tensored spin matrices  $\mathcal{B}^{\otimes n} = \{\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n} \mid 0 \leq i_j \leq 3\}$  form an orthonormal basis which we will call the spin basis. The standard basis of matrix units of  $M_{2^n}$  consists of the tensor products of the matrix units of  $M_2$ . The map  $C_{\mathcal{B}^{\otimes n}} : M_{2^n} \rightarrow M_{2^n}^d$  taking the standard basis of matrix units to this spin basis is then the tensor product of the maps on each factor  $M_2$ , so  $(C_{\mathcal{B}^{\otimes n}})(C_{\mathcal{B}^{\otimes n}})^T$  will be the transpose map on  $M_{2^n}$ . Thus the map from the spin basis on  $M_{2^n}$  to its dual basis will also be a co-positive order isomorphism.

Again applying Corollary ?? yields that a map,  $\Psi : M_{2^n} \rightarrow M_p$  is completely positive if and only if

$$\sum_{i_1, \dots, i_n=0}^3 \Psi(\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n}) \otimes \sigma_{i_1}^t \otimes \cdots \otimes \sigma_{i_n}^t$$

is a positive  $2^n p \times 2^n p$  matrix.

Similarly,  $\Psi$  is completely co-positive if and only if

$$\sum_{i_1, \dots, i_n=0}^3 \Psi(\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n}) \otimes \sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n}$$

is a positive  $2^n p \times 2^n p$  matrix.

□

For our final application we study the map from the Weyl basis to its dual basis. We will compute the duality map for the Weyl basis, with the conclusion that this map is a complete order isomorphism for  $n = 2$ , but is not an order isomorphism for  $n > 2$ . Below  $n > 1$  is a positive integer, and all indices are viewed as members of  $\mathbb{Z}_n$ .

*Definition 16.* Let  $e_0, \dots, e_{n-1}$  be the standard basis of  $\mathbb{C}^n$ , and  $\mathcal{B} = \{E_{ab} \mid a, b \in \mathbb{Z}_n\}$  the corresponding matrix units. Let  $U, V \in M_n$  be defined by  $Ve_j = z^j e_j$  and  $Ue_j = e_{j+1}$  where  $z = \exp(2\pi i/n)$ . Then  $\{\frac{1}{\sqrt{n}}U^a V^b \mid a, b \in \mathbb{Z}_n\}$  is an orthonormal basis for  $M_n$  which we call the *Weyl basis*  $\mathcal{W}$ .

The unitary matrices  $\{U^a V^b \mid a, b \in \mathbb{Z}_n\}$  are usually called the *discrete Weyl matrices* or the *generalized Pauli matrices*.

**Lemma 17.** Define  $C_{\mathcal{W}} \in L(M_n)$  by  $C_{\mathcal{W}}(E_{ab}) = \frac{1}{\sqrt{n}}U^a V^b$ . With respect to the standard basis of matrix units, we have the following matrix entries for  $C_{\mathcal{W}}$  and  $C_{\mathcal{W}}C_{\mathcal{W}}^T$ :

$$[C_{\mathcal{W}}]_{ab,cd} = z^{db}\delta_{b+c,a} \quad \text{and} \quad [C_{\mathcal{W}}C_{\mathcal{W}}^T]_{ab,cd} = \delta_{b,-d}\delta_{a,c-2d}.$$

*Proof.* We have  $U^a V^b e_j = z^{bj} E_{j+a,j} e_j$  so

$$U^a V^b = \sum_j z^{bj} E_{j+a,j}.$$

Thus

$$\begin{aligned} [C_{\mathcal{W}}]_{ab,cd} &= \langle C_{\mathcal{W}}(E_{cd}), E_{ab} \rangle \\ &= \frac{1}{\sqrt{n}} \langle U^c V^d, E_{ab} \rangle \\ &= \frac{1}{\sqrt{n}} \langle \sum_j z^{dj} E_{j+c,j}, E_{ab} \rangle \\ &= \frac{1}{\sqrt{n}} \sum_j z^{dj} \delta_{j+c,a} \delta_{j,b} \\ &= \frac{1}{\sqrt{n}} z^{db} \delta_{b+c,a} \end{aligned} \tag{8}$$

Now

$$[C_{\mathcal{W}}C_{\mathcal{W}}^T]_{ab,cd} = \sum_{jk} [C_{\mathcal{W}}]_{ab,jk} [C_{\mathcal{W}}^T]_{jk,cd} = \sum_{jk} [C_{\mathcal{W}}]_{ab,jk} [C_{\mathcal{W}}]_{cd,jk}.$$

In the first factor  $[C_{\mathcal{W}}]_{ab,jk}$  of the last sum we use the expression (??) for  $[C_{\mathcal{W}}]_{ab,cd}$  with the substitutions  $c \rightarrow j$  and  $d \rightarrow k$ . In the second factor  $[C_{\mathcal{W}}]_{cd,jk}$  we use (??) with the

substitutions  $a \rightarrow c, b \rightarrow d, c \rightarrow j, d \rightarrow k$ . We get

$$[C_{\mathcal{W}}C_{\mathcal{W}}^T]_{ab,cd} = \frac{1}{n} \sum_{jk} z^{kb} \delta_{b+j,a} z^{kd} \delta_{d+j,c}.$$

The summands will be nonzero if and only if  $j = a - b = c - d \pmod{n}$ . Thus

$$[C_{\mathcal{W}}C_{\mathcal{W}}^T]_{ab,cd} = \frac{1}{n} \delta_{a-b,c-d} \sum_k z^{k(b+d)}.$$

The sum will be zero unless  $b + d = 0$ , in which case it has the value  $n$ . Thus

$$[C_{\mathcal{W}}C_{\mathcal{W}}^T]_{ab,cd} = \delta_{a-b,c-d} \delta_{b+d,0} = \delta_{b,-d} \delta_{a,c-2d}.$$

□

Note that Lemma ?? gives

$$(C_{\mathcal{W}}C_{\mathcal{W}}^T)(E_{c,d}) = E_{c-2d,-d}, \quad (9)$$

so in particular  $C_{\mathcal{W}}C_{\mathcal{W}}^T$  acts as a permutation on the basis of matrix units.

**Corollary 18.** *For the Weyl basis  $\mathcal{W}$ , the duality map  $\mathcal{D}_{\mathcal{W}}$  is a complete order isomorphism if  $n = 2$ , and is not an order isomorphism for  $n > 2$ .*

*Proof.* If  $n = 2$ , then from (??)  $C_{\mathcal{W}}C_{\mathcal{W}}^T$  is the identity map, and hence  $\mathcal{D}_{\mathcal{W}}$  is a complete order isomorphism.

Now let  $n > 2$ . Suppose first (to reach a contradiction) that  $C_{\mathcal{W}}C_{\mathcal{W}}^T = \Phi_C$  for some invertible  $C \in L(M_n)$ . Then by (??),

$$E_{-d,-d} = (C_{\mathcal{W}}C_{\mathcal{W}}^T)(E_{dd}) = \Phi_C E_{dd} = R_{C e_d, C e_d}.$$

Thus for all  $d$  there are scalars  $\lambda_d$  of modulus one such that  $C e_d = \lambda_d e_{-d}$ . Then

$$\begin{aligned} E_{c-2d,-d} &= (C_{\mathcal{W}}C_{\mathcal{W}}^T)(E_{cd}) = \Phi_C(E_{cd}) \\ &= R_{C e_c, C e_d} = \lambda_c \bar{\lambda}_d E_{-c,-d}. \end{aligned} \quad (10)$$

This implies  $c - 2d = -c$ , so  $2c = 2d \pmod{n}$  for all  $c, d$ . This is impossible for  $n > 2$ .

Now suppose  $C_{\mathcal{W}}C_{\mathcal{W}}^T = t \circ \Phi_C$ . Then again applying (??),

$$\begin{aligned} E_{-d,-d} &= (C_{\mathcal{W}}C_{\mathcal{W}}^T)(E_{d,d}) = (\Phi_C(E_{d,d}))^t \\ &= (R_{C e_d, C e_d})^t = (R_{\overline{C e_d}, \overline{C e_d}}). \end{aligned} \quad (11)$$

This implies that for all  $d$ ,  $\overline{Ce_d}$  is a multiple of  $e_{-d}$ , and hence  $Ce_d$  is a multiple of  $\overline{e_{-d}} = e_{-d}$ .  
As above

$$\begin{aligned} E_{c-2d,-d} &= (C_W C_W^T)(E_{cd}) = (R_{C_{e_c}, C_{e_d}})^t \\ &= R_{\overline{C_{e_d}}, \overline{C_{e_c}}} = \lambda_c \bar{\lambda}_d E_{-c,-d}. \end{aligned} \tag{12}$$

This implies  $c - 2d = -c$  for all  $c, d$ , which again is impossible for  $n > 2$ . □

*Remark 19.* The Weyl basis for  $n = 2$  is slightly different than the Pauli spin basis. Indeed, one has

$$\begin{aligned} \frac{1}{\sqrt{2}}I &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & \frac{1}{\sqrt{2}}U &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \frac{1}{\sqrt{2}}V &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, & \frac{1}{\sqrt{2}}UV &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

These are the Pauli spin matrices except for normalization and a missing factor of  $i$  in the last. Again, applying Corollary ?? yields the usual Choi condition.

Recall that for the Pauli spin matrices we found  $C_B C_B^T$  was the transpose map, so  $\mathcal{D}_B$  in that case was co-positive.

*Remark 20.* Note that for  $M_{2^n}$  if we take tensors of the Weyl basis for  $M_2$ , then we will get another basis for which the duality map is a complete order isomorphism.

## THE CONJUGATE LINEAR DUALITY MAP

Using the fact that  $M_n$  is a Hilbert space, we also have a canonical conjugate linear isomorphism between  $M_n$  and its dual space. This map is unaffected by whether we make the inner product conjugate linear in the first or second variable, so we use the physics convention that inner products are conjugate linear in the first variable. Thus, the inner product on  $M_n$  can be given by

$$\langle A, B \rangle = \text{tr}(A^* B)$$

and the conjugate linear Hilbert space duality map is given by

$$\mathcal{D}_d : M_n \rightarrow M_n^d \text{ where } \mathcal{D}_d(A)(B) = \text{tr}(A^* B).$$



The inverse of this map

$$\Gamma_d = \mathcal{D}_d^{-1} : M_n^d \rightarrow M_n$$

sends the linear functional  $f_A(B) = \text{tr}(A^*B)$  to the matrix  $A$  which is the adjoint (i.e., conjugate transpose) of the density matrix.

**Proposition 21.** *The duality maps  $\mathcal{D}_d$  and  $\Gamma_d$  are conjugate linear complete order isomorphisms.*

*Proof.* By Corollary ?? the linear map that sends a functional to its density matrix is a co-positive order isomorphism. Hence, the map that sends a functional to the transpose of its density matrix is a complete order isomorphism. But a matrix  $(c_{ij})$  is positive if and only if the matrix  $(\overline{c_{ij}})$  is positive. Thus, the duality map  $\Gamma_d$ , which sends a functional to the adjoint of its density matrix is a complete order isomorphism. Consequently, so is its inverse  $\mathcal{D}_d$ .  $\square$

The above result has a nice interpretation in terms of bases. Choi's characterization says that a map  $\Phi : M_n \rightarrow M_p$  is completely positive iff the matrix  $C_\Phi$  defined in (??) is positive. As observed in Example ??, in the definition of  $C_\Phi$ , the basis  $\{E_{ij}\}$  can't be replaced by an arbitrary orthonormal basis. The following result provides an alternate description of the Choi matrix that does have this independence property. Recall that for a matrix  $B = (b_{ij})$  we set  $\overline{B} = (\overline{b_{ij}})$ .

**Proposition 22.** *Let  $\{B_l\}_{l=1}^{n^2}$  be an orthonormal basis for  $M_n$ . A complex linear map  $\Phi : M_n \rightarrow M_p$  is completely positive if and only if*

$$\sum_{l=1}^{n^2} \overline{B}_l \otimes \Phi(B_l) \tag{13}$$

*is a positive  $np \times np$  matrix. The matrix in (??) is independent of the choice of orthonormal basis, and equals the Choi matrix  $C_\Phi$ .*

*Proof.* Let  $f_A \in M_n^d$  be given by  $f_A(B) = \text{tr}(A^*B)$ , so that

$$\Gamma_d(f_A) = A = \sum_{l=1}^{n^2} \langle B_l, A \rangle B_l = \sum_{l=1}^{n^2} \overline{f_A(B_l)} B_l.$$

Thus, with respect to this basis

$$\Gamma_d(f) = \sum_{l=1}^{n^2} \overline{f(B_l)} B_l \quad \text{for all } f \in M_n^d.$$

Let  $(f_{ij}) \in M_n^d$  be the matrix defined by  $\Phi(A) = (f_{ij}(A))$  for  $A \in M_n$ . Recall that by definition, the matrix  $(f_{ij})$  is positive iff  $\Phi$  is completely positive. Using the fact that  $\Gamma_d$  is a complete order isomorphism, we have that  $\Phi$  is completely positive if and only if

$$(\Gamma_d(f_{ij})) = \sum_{l=1}^{n^2} \overline{(f_{ij}(B_l)B_l)} = \sum_{l=1}^{n^2} \overline{\Phi(B_l)} \otimes B_l \quad (14)$$

is a positive  $np \times np$  matrix. Using that fact that a matrix is positive if and only if its complex conjugate matrix is positive, the proposition now follows by applying the  $*$ -isomorphism that takes  $A \otimes B$  to  $B \otimes A$ .

Finally, since the matrix  $(f_{ij}) \in M_n^d$  is determined by  $\Phi$ , the matrix  $\sum_l \overline{B_l} \otimes \Phi(B_l)$  is independent of the choice of orthonormal basis  $\{B_l\}$ . For the standard basis  $\{E_{ij}\}$  the matrix (??) is just the Choi matrix, and hence the matrix in (??) equals the Choi matrix for all orthonormal bases  $\{B_l\}$ .  $\square$

Note that the matrix in (??) is the partial transpose of the matrix  $\mathcal{J}(\Phi)$  defined by Jamiołkowski, cf. (??).

## Acknowledgements

The research on this paper was begun during the program *Operator structures in quantum information theory* at the Banff International Research Station.

## REFERENCES

- <sup>1</sup>E. Alfsen and F. Shultz, *State spaces of operator algebras: basic theory, orientations, and  $C^*$ -products*, Mathematics: Theory & Applications, Birkhäuser Boston, 2001.
- <sup>2</sup>M.D. Choi, Completely positive linear maps on complex matrices, *Linear Algebra and Appl.* **10**(1975), 285-290.
- <sup>3</sup>V. Paulsen, I. Todorov, M. Tomforde, Operator system structures on ordered spaces, *Proc. London Math. Soc.*(2011) 102(1), p 25-49.
- <sup>4</sup>A. Jamiołkowski, Linear transformations which preserve trace and the positive semidefiniteness of operators, *Reports on Mathematical Physics* **3** (1972) 275–278.
- <sup>5</sup>R. Kadison, Isometries of operator algebras, *Annals of Mathematics* (1951) **54** 325–338.

<sup>6</sup>V. Paulsen, *Completely bounded maps and operator algebras*, Cambridge Studies in Advanced Mathematics **78**, Cambridge University Press, 2003.