On Birkhoff's Theorem for Doubly Stochastic Completely Positive Maps of Matrix Algebras

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Dedicated to Karl Kraus (1938–1988).

ABSTRACT

A study is made of the extreme points of the convex set of doubly stochastic completely positive maps of the matrix algebra $\mathbb{M}_n$. If $n = 2$ the extreme points are precisely the unitary maps, but if $n \geqslant 3$ there are nonunitary extreme points, examples of which are exhibited. A tilde operation is defined on the linear maps of $\mathbb{M}_n$ and used to give an elementary derivation of a result of Kummerer and Maassen.

1. INTRODUCTION

Let $\mathbb{M}_n$ denote the *-algebra of $n \times n$ complex matrices, where * is hermitian conjugation. A $\mathbb{C}$-linear map $\phi : \mathbb{M}_n \to \mathbb{M}_n$ is

(1) *hermitian* if ϕ maps hermitian matrices to hermitian matrices,
(2) *positive* if ϕ maps positive matrices to positive matrices,
(3) *m-positive* if $\phi \otimes \mathrm{Id}$ is positive on $\mathbb{M}_n \otimes \mathbb{M}_m$, where Id is the identity map, $\mathbb{M}_m \to \mathbb{M}_m$,
(4) *completely positive* if ϕ is m-positive for every m.

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The positive map ϕ is

(1) *stochastic* if $\phi(\mathbb{1}) = \mathbb{1}$, where $\mathbb{1}$ denote the identity matrix,
(2) *doubly stochastic* if ϕ is stochastic and trace preserving:

$$\operatorname{Tr} \phi(A) = \operatorname{Tr} A \qquad \text{for all} \quad A \in \mathbb{M}_n .$$

According to Wigner's theorem, the invertible stochastic maps[1] are either unitary or antiunitary:

WIGNER'S THEOREM [1, Section 2.3]. *An invertible stochastic map is either*

(1) unitary, $\phi_U(A) = U^*AU$ *for some unitary* $U \in \mathbb{M}_n$ (*a unitary map is doubly stochastic and completely positive*) *or*

(2) antiunitary, $\psi_U(A) = U^*A^TU$ *for some unitary* $U \in \mathbb{M}_n$, *where* A^T *is the transpose of* A (*an antiunitary map is doubly stochastic but not completely positive*).

The set of doubly stochastic maps forms a compact convex subset of the set of all linear maps of $\mathbb{M}_n$. This is also the case for the set of doubly stochastic completely positive maps. Hence for either subset, any element is a finite convex sum of extreme points of the respective convex set.

An invertible stochastic map is extremal in the stochastic maps and therefore extremal in the doubly stochastic maps [2]. Tregub considers the question whether the invertible stochastic maps exhaust the extremal doubly stochastic maps.

TREGUB'S THEOREM [2].

(1) *The extremal doubly stochastic maps of* $\mathbb{M}_2$ *consist precisely of the invertible maps. Hence every doubly stochastic map of* $\mathbb{M}_2$ *is a convex combination of unitary and antiunitary maps.*

(2) *If* $n \geqslant 3$, *there are doubly stochastic maps which are not convex combinations of invertible maps. Hence there are noninvertible extremal doubly stochastic maps.*

We prove the analog of Tregub's theorem for the case of doubly stochastic *completely* positive maps.

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[1] By an invertible stochastic map is meant a stochastic map which has an inverse which is also stochastic.

THEOREM 1.

(1) *The extremal doubly stochastic completely positive maps of* $\mathbb{M}_2$ *consist precisely of the unitary maps. Hence every doubly stochastic completely positive map of* $\mathbb{M}_2$ *is a convex combination of unitary maps.*

(2) *If* $n \geqslant 3$, *there are nonunitary extremal doubly stochastic completely positive maps.*

An example of (2) is

$$\phi(A) = \frac{1}{j(j+1)} \sum_{\alpha=1}^{3} J^{(\alpha)} A J^{(\alpha)},$$

where $J^{(\alpha)}$ generate rotations about three orthogonal axes in the irreducible unitary representation of SU(2) of dimension $n = 2j + 1$.

Tregub's theorem and Theorem 1 show that the analog of the classical Birkhoff theorem for commutative algebras extends to the noncommutative case if $n = 2$ but not if $n \geqslant 3$.

BIRKHOFF'S THEOREM [3]. *The extremal doubly stochastic matrices are precisely the permutations. Hence every doubly stochastic matrix is a convex combination of permutations.*

For the case $n \geqslant 4$ the existence of nonunitary extremal doubly stochastic completely positive maps of $\mathbb{M}_n$ is already contained in the work of Tregub [2] and Kummerer and Maassen [4]. Tregub constructs a nonunitary extremal diagonal map of $\mathbb{M}_4$. Diagonal maps are considered in Section 3, and Tregub's example in Section 4.3. Using Hunt's characterization of the generators of convolution semigroups, Kummerer and Maassen construct examples of diagonal semigroups which are not convex combinations of unitary maps if $n \geqslant 4$. In Section 6 we present an elementary derivation of their result using the tilde technique defined in Section 5.

The tilde technique is formulated using the one-one correspondence between linear maps of $\mathbb{M}_n$ into itself on the one hand and linear functionals on $\mathbb{M}_n \otimes \mathbb{M}_n$ on the other [5–10]. In Section 5 we give a useful form of this correspondence and derive the relation between the restriction of the linear functional to each of the subalgebras $\mathbb{M}_n \otimes \mathbb{1}$ and $\mathbb{1} \otimes \mathbb{M}_n$ and the properties of the linear map ϕ. In particular (Remark 11) there is a one-one correspondence between doubly stochastic completely positive maps of $\mathbb{M}_n$ and doubly chaotic states on $\mathbb{M}_n \otimes \mathbb{M}_n$, the unitary maps corresponding to doubly chaotic vector states. (Doubly chaotic vector states occur for example in the EPR experiment [11], where a pure state on $\mathbb{M}_2 \otimes \mathbb{M}_2$ (the state of two spins) reduces on $\mathbb{M}_2 \otimes \mathbb{1}$ and on $\mathbb{1} \otimes \mathbb{M}_2$ to totally unpolarized states.)

1.1. *Conventions*

An element A of the algebra $\mathbb{M}_n$ is associated with a linear functional F_A on $\mathbb{M}_n$ by the formula

$$F_A(B) = \mathrm{Tr}(AB) \qquad \text{for all} \quad B \in \mathbb{M}_n,$$

and any linear functional is uniquely represented in this manner. Hence the canonical pairing of $\mathbb{M}_n$ and its dual is converted into a bilinear form $(\cdot, \cdot): \mathbb{M}_n \times \mathbb{M}_n \to \mathbb{C}$; thus $F_A(B) = \mathrm{Tr}(AB) = (A, B) = (B, A)$. We will write Δ for the inverse of the map $A \to F_A$, so that if f is a linear functional, Δf is the matrix such that $F_{\Delta f} = f$. A *state* is a positive linear functional f with $f(\mathbb{1}) = 1$. In this case Δf is a density matrix, that is, a normalized positive matrix: $\Delta f \geqslant 0$, $\mathrm{Tr}\,\Delta f = 1$. We will denote the tracial state by ω; it is the "totally chaotic" state given by $\omega(A) = n^{-1}\,\mathrm{Tr}\,A$, $A \in \mathbb{M}_n$. In quantum theory this has the interpretation as the totally unpolarized state, the microcanonical state, or the state at infinite temperature. We note that $\Delta\omega = n^{-1}\,\mathbb{1}$.

If ϕ is a linear map of $\mathbb{M}_n$ into itself, the transposed map ϕ^t is defined by

$$(\phi^t(A), B) = (A, \phi(B)) \tag{1}$$

Then ϕ^t is positive if and only if ϕ is. Since for $m = 1, 2, \ldots, \mathbb{M}_n \otimes \mathbb{M}_m$ is of type I, it has a unique normalized trace, tr, putting it into linear correspondence with its dual. The transpose thus defined will also be denoted ^{t}. One then easily sees that $(\phi \otimes \mathrm{Id})^t = \phi^t \otimes \mathrm{Id}$. It follows that if ϕ is completely positive, so is ϕ^t. Then ϕ is doubly stochastic if and only if ϕ and ϕ^t are stochastic. Furthermore, let $K, L \in \mathbb{M}_n$; we define

(i) $\mathrm{CP}_n(K) = \{\phi : \phi$ is a completely positive map of $\mathbb{M}_n$ and $\phi(\mathbb{1}) = K\}$,
(ii) $\mathrm{CP}_n(K, L) = \{\phi : \phi \in \mathrm{CP}_n(K)$ and $\phi^t(\mathbb{1}) = L\}$.

If follows from Equation (1) that $\mathrm{Tr}\,K = \mathrm{Tr}\,L$, and this is also a sufficient condition for $\mathrm{CP}_n(K, L)$ to be nonempty if K and L are positive. More precisely,

PROPOSITION 1. *Let* $K, L \in \mathbb{M}_n$ *be such that* $\mathrm{Tr}\,K = \mathrm{Tr}\,L$. *Then*

(1) *there exists a linear map* $\phi: \mathbb{M}_n \to \mathbb{M}_n$ *such that* $\phi(\mathbb{1}) = K$, $\phi^t(\mathbb{1}) = L$;
(2) *if* K *and* L *are hermitian, then* ϕ *may be taken hermitian;*
(3) *if* K *and* L *are positive, then* ϕ *may be taken completely positive.*

Proof. To prove (1) write $K = K_1 + iK_2$, $L = L_1 + iL_2$, where K_j, L_j are hermitian for $j = 1, 2$. Then $\mathrm{Tr}\,K_j = \mathrm{Tr}\,L_j$ and, given (2), there exist ϕ_j

such that $\phi_j(\mathbb{1}) = K_j$, $\phi_j^t(\mathbb{1}) = L_j$. Hence $\phi = \phi_1 + i\phi_2$ has the required properties.

To prove (2) write $K = K_1 - K_2$, $L = L_1 - L_2$, where K_j, L_j are positive for $j = 1, 2$. Suppose $\operatorname{Tr} K_1 \geqslant \operatorname{Tr} L_1$. Then there exists $\varepsilon \geqslant 0$ such that $\operatorname{Tr} K_1 = \operatorname{Tr}(L_1 + \varepsilon \mathbb{1})$ and hence $\operatorname{Tr} K_2 = \operatorname{Tr}(L_2 + \varepsilon \mathbb{1})$. Given (3), there exist hermitian ϕ_j such that $\phi_j(\mathbb{1}) = K_j$ and $\phi_j^t(\mathbb{1}) = (L_j + \varepsilon \mathbb{1})$. Then $\phi = \phi_1 - \phi_2$ has the required properties. A similar proof applies to the case $\operatorname{Tr} K_1 \leqslant \operatorname{Tr} L_1$.

To prove (3) note that the completely positive map $\phi = \tau^{-1} \operatorname{Tr}(L\,\cdot\,)\,K$, where $\tau = \operatorname{Tr} K = \operatorname{Tr} L$, has the required properties. ∎

We observe that the map ϕ constructed in the proof corresponds to a product functional on $\mathbb{M}_n \otimes \mathbb{M}_n$ [Equation (6)].

2. EXTREMALITY CONDITION FOR DOUBLY STOCHASTIC COMPLETELY POSITIVE MAPS

For any $V \in \mathbb{M}_n$ the map $\phi_V = V^* \cdot V$ [i.e $\phi_V(A) = V^*AV$] is completely positive, and every completely positive map of $\mathbb{M}_n$ is a sum of such maps [12–14]:

$$\phi = \sum_{\alpha=1}^{a} V^{(\alpha)*} \cdot V^{(\alpha)}. \tag{2}$$

The representation (2) is not unique, but the matrices $V^{(\alpha)}$ may always be taken linearly independent, and in that case the number a of terms is uniquely determined, and furthermore, if

$$\phi = \sum_{\beta=1}^{b} W^{(\beta)*} \cdot W^{(\beta)}$$

is any other representation for ϕ, then

$$W^{(\beta)} = \sum_{\alpha=1}^{a} S_{\beta\alpha} V^{(\alpha)}, \tag{3}$$

where $S : \mathbb{C}^a \to \mathbb{C}^b$ is isometric: $S^*S = \mathbb{1}_a$, the identity map on $\mathbb{C}^a$. If the matrices $W^{(\beta)}$ are also linearly independent, then S is unitary. (For a discussion of these points see Choi [12].)

The extreme points of the convex set $\mathrm{CP}_n(K, L)$ can be characterized by a property of the matrices $V^{(\alpha)}$ entering into the representation (2) for the completely positive map ϕ, in close analogy with Choi's characterization of the extreme points of $\mathrm{CP}_n(K)$ [12]. Choi's characterization is given in the following theorem.

CHOI'S THEOREM [12]. *The map ϕ is extreme in $\mathrm{CP}_n(K)$ if and only if ϕ admits an expression of the form (2) where*

$$\sum_{\alpha=1}^{a} V^{(\alpha)*}V^{(\alpha)} = K$$

and

$$\{V^{(\alpha)*}V^{(\beta)}\}_{\alpha,\beta=1,\ldots,a}$$

is a linearly independent set of matrices.

REMARK 1. The linear independence of $\{V^{(\alpha)}\}_{\alpha=1,\ldots,a}$ follows from the linear independence of $\{V^{(\alpha)*}V^{(\beta)}\}_{\alpha,\beta=1,\ldots,a}$.

In order to state the characterization of the extreme points of $\mathrm{CP}_n(K, L)$ the following definition is needed.

DEFINITION 1. The pairs $(u_1, v_1), \ldots, (u_N, v_N)$ of elements of a linear space are said to be biindependent if

$$\sum_{j=1}^{N} c_j u_j = 0 \quad \text{and} \quad \sum_{j=1}^{N} c_j v_j = 0$$

imply $c_j = 0$ for all $j = 1, 2, \ldots, N$. The N pairs of elements will be denoted $u_1, \ldots, u_N; v_1, \ldots, v_N$ (the relative order of the u's and v's being fixed).

REMARK 2. Clearly, the pairs $(u_1, v_1), \ldots, (u_N, v_N)$ of vectors in $\mathbb{C}^r$ are biindependent if and only if $u_1 \oplus v_1, \ldots, u_N \oplus v_N$ are linearly independent in $\mathbb{C}^{2r}$. If follows that $N \leqslant 2r$ if they are biindependent.

We may now state Theorem 2, the proof of which follows closely Choi's proof of Theorem 5 of [12] and will not be given here.

THEOREM 2. *The map ϕ is extreme in $\mathrm{CP}_n(K, L)$ if and only if ϕ admits an expression of the form* (2) *where*

$$\sum_{\alpha=1}^{a} V^{(\alpha)*}V^{(\alpha)} = K, \qquad \sum_{\alpha=1}^{a} V^{(\alpha)}V^{(\alpha)*} = L,$$

and

$$\left\{V^{(\alpha)*}V^{(\beta)}\right\}_{\alpha,\beta=1,\dots,a};\left\{V^{(\beta)}V^{(\alpha)*}\right\}_{\alpha,\beta=1,\dots,a}$$

is a biindependent set of matrices.

REMARK 3. Explicitly, the biindependence in Theorem 2 is expressed as follows:

$$\sum c_{\alpha\beta}V^{(\alpha)*}V^{(\beta)} = 0 \quad \text{and} \quad \sum c_{\alpha\beta}V^{(\beta)}V^{(\alpha)*} = 0$$

imply $c_{\alpha,\beta} = 0$ for all $\alpha, \beta = 1, 2, \dots, a$. According to Remark 2,

$$a^2 \leqslant 2n^2.$$

REMARK 4. The linear independence of $\{V^{(\alpha)}\}_{\alpha=1,\dots,a}$ follows from the biindependence of $\{V^{(\alpha)*}V^{(\beta)}\}_{\alpha,\beta=1,\dots,a}; \{V^{(\beta)}V^{(\alpha)*}\}_{\alpha,\beta=1,\dots,a}$.

As a special case of Theorem 2 we obtain

COROLLARY 1. *The map ϕ is extremal in the doubly stochastic completely positive maps of $\mathbb{M}_n$ if and only if ϕ admits a representation of the form* (2) *where*

$$\sum_{\alpha=1}^{a} V^{(\alpha)*}V^{(\alpha)} = \mathbb{1}, \qquad \sum_{\alpha=1}^{a} V^{(\alpha)}V^{(\alpha)*} = \mathbb{1},$$

and

$$\left\{V^{(\alpha)*}V^{(\beta)}\right\}_{\alpha,\beta=1,\dots,a};\left\{V^{(\beta)}V^{(\alpha)*}\right\}_{\alpha,\beta=1,\dots,a}$$

is a biindependent set of matrices.

3. DIAGONAL MAPS

A simple class of maps, which will provide examples in Sections 4 and 6, is given by the diagonal maps.

DEFINITION 2. A linear map ϕ of $\mathbb{M}_n$ into itself is *diagonal* if it has the form

$$\phi(A)_{jk} = C_{jk} A_{jk} \qquad \text{for all} \quad j, k = 1, 2, \ldots, n$$

for some $C \in \mathbb{M}_n$. The identity map is diagonal with $C = E$, where

$$E_{jk} = 1 \qquad \text{for all} \quad j, k = 1, 2, \ldots, n.$$

The following lemma is easily proved.

LEMMA 1. *If A and C are positive $n \times n$ matrices, then $\phi(A)$ of Definition 2 is positive.*

We then have

PROPOSITION 2. *The diagonal map ϕ (Definition 2) is positive if and only if C is positive. In this case ϕ is actually completely positive.*

Proof. If ϕ is positive, then $C = \phi(E)$ is positive, since E is positive. If C is positive, then ϕ is positive by Lemma 1. For any integer m, the map of $\mathbb{M}_n \otimes \mathbb{M}_m$ defined by $\hat{\phi} = \phi \otimes \mathrm{Id}$ is a diagonal map with $\hat{C} = C \otimes E$. If C is positive, then $\hat{C}$ is positive and thus $\hat{\phi}$ is positive. Hence ϕ is completely positive. ∎

REMARK 5. If ϕ is diagonal, then ϕ^t is also diagonal with C replaced by its transpose. Thus $\phi(\mathbb{1}) = \phi^t(\mathbb{1}) = K$, where $K_{jk} = C_{jj}\delta_{jk}$, $j, k = 1, \ldots, n$. Thus ϕ is stochastic if and only if $C_{jj} = 1$ for all $j = 1, \ldots, n$, and then ϕ is doubly stochastic.

PROPOSITION 3. *If ϕ is a completely positive diagonal map, then in any representation (2) the matrices $V^{(\alpha)}$ are diagonal.*

Proof. From the representation (2) we conclude

$$\sum_{\alpha, i, m} \overline{V_{ij}^{(\alpha)}} A_{im} V_{mk}^{(\alpha)} = C_{jk} A_{jk}.$$

Since A is arbitrary,

$$\sum_{\alpha} \overline{V_{ij}^{(\alpha)}} V_{mk}^{(\alpha)} = C_{jk} \delta_{ij} \delta_{mk}.$$

Setting $i = m$, $j = k$, $i \neq j$, we obtain

$$\sum_{\alpha} |V_{ij}^{(\alpha)}|^2 = 0.$$

Thus $V_{ij}^{(\alpha)} = 0$ if $i \neq j$. ■

We may then write

$$V_{jk}^{(\alpha)} = \lambda_j^{(\alpha)} \delta_{jk} \tag{4}$$

and

$$C_{jk} = \sum_{\alpha} \overline{\lambda_j^{(\alpha)}} \lambda_k^{(\alpha)}. \tag{5}$$

The extremality condition, Theorem 1, may be formulated in the case of diagonal maps with the aid of the following definition.

DEFINITION 3. The elements $u_1, \ldots, u_N$ of $\mathbb{C}^r$ are said to form a *full* set of vectors if

$$(u_j, Au_j) = 0 \quad \text{for all } j = 1, \ldots, N \quad \text{implies} \quad A = 0.$$

Here $A \in \mathbb{M}_r$, and (u, v) is the usual scalar product in $\mathbb{C}^r$.

We may then state

THEOREM 3. *The following conditions on the completely positive diagonal map ϕ are equivalent:*

(i) *ϕ is extremal in $\mathrm{CP}_n(K, K)$, where K is given in Remark* 5.

(ii) *ϕ is extremal in $\mathrm{CP}_n(K)$.*

(iii) *The matrix C (Definition 2) may be expressed as $C_{jk} = \sum_{\alpha=1}^{a} \overline{\lambda_j^{(\alpha)}} \lambda_k^{(\alpha)}$, where $\sum_{\alpha, \beta} b_{\alpha\beta} \lambda_j^{(\alpha)} \lambda_j^{(\beta)} = 0$ for all $j = 1, 2, \ldots, n$ implies $b = 0$.*

(iv) *ϕ has the representation (2) where $V_{jk}^{(\alpha)} = \lambda_j^{(\alpha)} \delta_{jk}$, and the vectors $u_1, \ldots, u_n$ are a full set of vectors in $\mathbb{C}^a$, where $(u_j)_\alpha = \lambda_j^{(\alpha)}$.*

REMARK 6. The linear independence of the diagonal matrices $\{V^{(\alpha)*}V^{(\beta)}\}_{\alpha,\beta=1,\ldots,a}$ implies $a^2 \leqslant n$, since n is the dimension of the space of diagonal $n \times n$ matrices.

Proof of Theorem 3. According to Proposition 3, the matrices $V^{(\alpha)}, V^{(\alpha)*}$ occurring in the representation (2) are diagonal and thus mutually commuting. It follows that the biindependence expressed in Theorem 1 is in this case equivalent to the linear independence expressed in Choi's theorem. Thus (i) and (ii) are equivalent. The matrix $V^{(\alpha)*}V^{(\beta)}$ is diagonal with diagonal entries $\overline{\lambda_j^{(\alpha)}}\lambda_j^{(\beta)}$. Thus the linear independence of these matrices is equivalent to the condition in (iii), where C is related to $V^{(\alpha)}$ by Equations (4) and (5). The condition in (iii) expresses the fullness (Definition 3) of $u_1, \ldots, u_n$ in $\mathbb{C}^a$. ∎

DEFINITION 4. The linear maps ϕ_1 and ϕ_2 of $\mathbb{M}_n$ into itself are unitarily equivalent if there are unitary maps $\phi_R = R^* \cdot R$, $\phi_S = S^* \cdot S$ such that $\phi_2 = \phi_R \phi_1 \phi_S$.

Unitary equivalence preserves complete positivity, stochasticity, and extremality. If ϕ_1 and ϕ_2 are unitarily equivalent, then $K_2 = R^* K_1 R$ and $L_2 = S L_1 S^*$, and their representations (2) satisfy $V_2^{(\alpha)} = S V_1^{(\alpha)} R$.

THEOREM 4.

(1) *If ϕ is completely positive with representation* (2) *where $a = 1$, then ϕ is unitarily equivalent to a completely positive diagonal map.*

(2) *If ϕ is a doubly stochastic completely positive map with representation* (2) *where $a = 2$, then ϕ is unitarily equivalent to a doubly stochastic completely positive diagonal map.*

Proof. (1): Any matrix $V \in \mathbb{M}_n$ can be expressed as the product of a unitary matrix and a positive matrix (polar decomposition). The positive matrix can be diagonalized with a unitary matrix. We may then write $V = SDR$, where S, R are unitary and D is a positive diagonal matrix. Now if ϕ has the representation (2) with $a = 1$, then expressing $V^{(1)} = SDR$, we have $\phi = \phi_R \phi' \phi_S$, where ϕ' is a completely positive diagonal map.

(2): If ϕ has the representation (2) with $a = 2$, then express $V^{(1)} = SDR$ and define W by $V^{(2)} = SWR$. Then $\phi = \phi_R \phi' \phi_S$, where ϕ' is a doubly stochastic completely positive map with $V'^{(1)} = D$, $V'^{(2)} = W$. Then $D^2 + W^*W = \mathbb{1}$, $D^2 + WW^* = \mathbb{1}$. It follows that W is normal: $WW^* = W^*W$. A polar decomposition for W gives $W = UT$, where U is unitary and T is positive; that W is normal implies that U and T commute. Then $D^2 + T^2 = \mathbb{1}$. It follows that $T = (\mathbb{1} - D^2)^{1/2}$, which is diagonal, and that U commutes with D and can thus be simultaneously diagonalized with D. We thus obtain ϕ'' which is unitarily equivalent to ϕ and is diagonal. ■

4. ON BIRKHOFF'S THEOREM

In this section we consider the extreme points of the doubly stochastic completely positive maps of $\mathbb{M}_n$ for $n = 2, 3, 4$.

4.1. The case $n = 2$

If ϕ is an extremal doubly stochastic completely positive map of $\mathbb{M}_2$, then it has the representation (2). According to Remark 3, the biindependence in Theorem 2 requires $a^2 \leqslant 2n^2 = 8$, from which it follows that $a = 1$ or 2. If $a = 1$ then $\phi = V^* \cdot V$ and $V^*V = \mathbb{1}$, that is, V is unitary, so ϕ is a unitary map. If $a = 2$, according to Theorem 4 ϕ is unitarily equivalent to a diagonal map, which will also be extremal. But according to Remark 6 we must then have $a^2 \leqslant 2$. Thus only $a = 1$ is possible when $n = 2$, for an extremal map.

Thus, the set of extremal doubly stochastic completely positive maps of $\mathbb{M}_2$ consists of the unitary maps, and every doubly stochastic completely positive map of $\mathbb{M}_2$ is a convex combination of unitary maps. This proves Theorem 1(1).

4.2. The case $n = 3$

If ϕ is a doubly stochastic completely positive *diagonal* map of $\mathbb{M}_3$, then it can be written as a convex combination of extremal doubly stochastic completely positive maps, which, according to Proposition 3, must be diagonal. Then according to Remark 6 these extremal diagonal maps must have $a = 1$ and are thus unitary. Furthermore, any doubly stochastic completely positive map ϕ with representation (2) and $a = 2$ is unitarily equivalent to a diagonal map, according to Theorem 4. As this diagonal map is a convex combination of unitary maps, the same holds for ϕ and we have proven

THEOREM 5.

(1) *If ϕ is a doubly stochastic completely positive* diagonal *map of $\mathbb{M}_3$, then it is a convex combination of diagonal unitary maps.*

(2) *If ϕ is a doubly stochastic completely positive map of $\mathbb{M}_3$ with representation* (2) *and $a = 2$, then ϕ is a convex combination of unitary maps.*

We can however construct a nonunitary extremal map ϕ of $\mathbb{M}_3$ with a representation (2) and $a = 3$, by setting $V^{(\alpha)} = (1/\sqrt{2})J^{(\alpha)}$, where

$$J^{(1)} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad J^{(2)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$

$$J^{(3)} = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}.$$

To see this note that $V^{(\alpha)*} = V^{(\alpha)}$ for all $\alpha = 1, 2, 3$ and $V^{(1)2} + V^{(2)2} + V^{(3)2} = \mathbb{1}$. Thus ϕ is doubly stochastic. We will show that the matrices $\{V^{(\alpha)}V^{(\beta)}\}_{\alpha,\beta=1,2,3}$ are linearly independent. It follows by Choi's theorem that ϕ is extremal in the stochastic maps and thus also extremal in the doubly stochastic maps (biindependence follows from linear independence). Now the matrices $J^{(\alpha)}$ transform according to the three-dimensional spin-$j = 1$ representation of SO(3) (the adjoint representation), and thus the matrices $T_{\alpha\beta} = J^{(\alpha)}J^{(\beta)} - \frac{2}{3}\delta_{\alpha\beta}\mathbb{1}$, $\alpha \leqslant \beta$, transform according to the five-dimensional $j = 2$ representation. The matrix $\mathbb{1} = \frac{1}{2}[J^{(1)2} + J^{(2)2} + J^{(3)2}]$ transforms according to the one-dimensional $j = 0$ (trivial) representation, and the matrices $S_{\alpha\beta} = [J^{(\alpha)}, J^{(\beta)}] = iJ^{(\gamma)}$ (α, β, γ cyclic permutations of $1, 2, 3$) transform according to the $j = 1$ representation. As these matrices are nonzero, they are necessarily linearly independent, since they transform according to inequivalent irreducible representations of SO(3). Hence $\{V^{(\alpha)}V^{(\beta)}\}_{\alpha,\beta=1,2,3}$ are linearly independent.

We observe that the above construction may be carried out for any irreducible representation of SO(3). In the $2j + 1$-dimensional spin-j representation the Casimir operator $J^{(1)2} + J^{(2)2} + J^{(3)2} = j(j+1)\mathbb{1}$. This proves Theorem 1(2).

4.3. *The case $n = 4$*

According to Remark 6, $n = 4$ is the smallest value of n such that nonunitary extremal doubly stochastic completely positive *diagonal* maps can exist. Then necessarily $a = 2$. An example may be constructed by setting

$$V^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix},$$

$$V^{(2)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{-i}{\sqrt{2}} \end{pmatrix}.$$

It is easily verified that $\{V^{(\alpha)*}V^{(\beta)}\}_{\alpha,\beta=1,2}$ are linearly independent, or equivalently (Theorem 3) that the vectors

$$u_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad u_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad u_3 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad u_4 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}$$

are a full set of vectors for $\mathbb{C}^2$. This gives Tregub's example [2].

We note that the maps given in Sections 4.2 and 4.3 are extremal not only in the doubly stochastic completely positive maps, but also in the stochastic completely positive maps.

5. THE TILDE OPERATION

The correspondence between linear maps of $\mathbb{M}_n$ into itself and linear functionals on $\mathbb{M}_n \otimes \mathbb{M}_n$ has been expressed in the literature in various forms [5–10]. Our approach is based on the formula

$$L_\phi(A \otimes B) = \omega\big(B^T\phi(A)\big) = \frac{1}{n}\operatorname{Tr} B^T\phi(A), \tag{6}$$

where B^T denotes the transpose of B, and ω is the tracial state. Equation (6) defines a one-one correspondence between the maps ϕ on $\mathbb{M}_n$ and the linear functionals L_ϕ on $\mathbb{M}_n \otimes \mathbb{M}_n$.

REMARK 7. The functional L_ϕ is normalized if and only if $\omega(\phi(\mathbb{1})) = 1$. That is, $L_\phi(\mathbb{1} \otimes \mathbb{1}) = 1$ if and only if $\operatorname{Tr}\phi(\mathbb{1}) = n$.

5.1. *Doubly Stochastic Maps and Doubly Chaotic States*

An interesting relation concerning the restriction of L_ϕ to each of the two factors $\mathbb{M}_n$ does not seem to have been previously noticed. Given a linear functional L on $\mathbb{M}_n \otimes \mathbb{M}_n$, let L' be the restriction of L to the first factor $\mathbb{M}_n \otimes \mathbb{1} \cong \mathbb{M}_n$, and L'' the restriction of L to the second factor $\mathbb{1} \otimes \mathbb{M}_n \cong \mathbb{M}_n$. That is,

$$L'(A) = L(A \otimes \mathbb{1}), \qquad L''(B) = L(\mathbb{1} \otimes B).$$

Thus L' and L'' are linear functionals on $\mathbb{M}_n$ and define elements $\Delta L'$ and $\Delta L'' \in \mathbb{M}_n$ under the pairing $(\cdot, \cdot)$ (Section 1.1). An easy computation based on Equation (6) gives

PROPOSITION 4.

$$\Delta L'_\phi = \phi^t(\Delta\omega) = n^{-1}\phi^t(\mathbb{1}),$$

$$\Delta L''_\phi = \phi(\Delta\omega)^T = n^{-1}\phi(\mathbb{1})^T.$$

It is useful to develop an explicit formula for the correspondence (6) relating linear maps and linear functionals. It is convenient to represent the $*$-algebra $\mathbb{M}_n \otimes \mathbb{M}_n$ faithfully as acting on the vector space $\mathbb{M}_n$ by $(A \otimes B)C = L_A R_{B^t} C = ACB^T$ $(A, B, C \in \mathbb{M}_n)$ extended by bilinearity to sums of elements of the form $\Sigma A \otimes B$. We introduce the scalar product $\langle A, B\rangle = n^{-1}\operatorname{Tr}(A^*B) = \omega(A^*B)$ on $\mathbb{M}_n$. This makes $\mathbb{M}_n$ into the Hilbert space of matrices with the Hilbert-Schmidt norm, and $\mathbb{M}_n \otimes \mathbb{M}_n$ is identified with $B(\mathbb{M}_n)$, the W^*-algebra of operators on $\mathbb{M}_n$. Define the linear functional $L_{C,D}$ on $\mathbb{M}_n \otimes \mathbb{M}_n$ by the formula $L_{C,D}(M) = \langle C, MD\rangle$ for $M \in \mathbb{M}_n \otimes \mathbb{M}_n = B(\mathbb{M}_n)$. Any linear functional on $\mathbb{M}_n \otimes \mathbb{M}_n$ may be expressed as a linear combination of such functionals. As for $\mathbb{M}_n$ in Section 1.1, every linear functional L on $\mathbb{M}_n \otimes \mathbb{M}_n$ corresponds to a matrix $\delta_L \in \mathbb{M}_n \otimes \mathbb{M}_n$ by the formula $L(M) = \operatorname{tr}(\delta_L M)$, where here tr is the trace on $\mathbb{M}_n \otimes \mathbb{M}_n$. Using Equation (6) we easily derive

PROPOSITION 5. *$L_{C,D}$ corresponds to the linear map $\phi_{C,D} = L_{C*}R_D = C^* \cdot D$ on $\mathbb{M}_n$.*

REMARK 8. The linear functional $L_{\mathbb{1},\mathbb{1}} = \langle \mathbb{1}, M\mathbb{1}\rangle$ is a state on $\mathbb{M}_n \otimes \mathbb{M}_n = B(\mathbb{M}_n)$, being the expectation in the unit vector $\mathbb{1} \in \mathbb{M}_n$. The corresponding density matrix $\delta L_{\mathbb{1},\mathbb{1}}$ is obviously $P_{\mathbb{1}} \in B(\mathbb{M}_n)$, the orthogonal projection onto $\mathbb{1} \in \mathbb{M}_n$. The linear map $\phi_{\mathbb{1},\mathbb{1}}$ corresponding to $L_{\mathbb{1},\mathbb{1}}$, given in Proposition 5, is the identity map of $\mathbb{M}_n$ onto itself.

We may obtain the following formula for the linear functional L_ϕ associated with the linear map ϕ:

$$L_\phi = L_{\mathbb{1},\mathbb{1}} \circ \hat{\phi}, \qquad \text{where} \quad \hat{\phi} = \phi \otimes \mathrm{Id}, \tag{7a}$$

or

$$\delta L_\phi = \hat{\phi}^t P_{\mathbb{1}} \tag{7b}$$

Here, the transpose map $\hat{\phi} \to \hat{\phi}^t$ is defined by

$$\mathrm{tr}[N\phi(M)] = \mathrm{tr}[\phi^t(N)M], \qquad M, N \in \mathbb{M}_n \otimes \mathbb{M}_n.$$

The expression (7) follows from

$$\begin{aligned} L_\phi(A \otimes B) = \omega(B^T\phi(A)) &= L_{\mathbb{1},\mathbb{1}}(\phi(A) \otimes B) \\ &= L_{\mathbb{1},\mathbb{1}}(\hat{\phi}(A \otimes B)). \end{aligned}$$

So

$$L_\phi = L_{\mathbb{1},\mathbb{1}} \circ \hat{\phi}.$$

Also,

$$\begin{aligned} L_{\mathbb{1},\mathbb{1}}(\hat{\phi}(A \otimes B)) &= \mathrm{tr}\left[P_{\mathbb{1}}\hat{\phi}(A \otimes B)\right] \\ &= \mathrm{tr}\left[(\hat{\phi}^t P_{\mathbb{1}})(A \otimes B)\right]. \end{aligned}$$

So

$$\delta_{L\phi} = \hat{\phi}^t P_{\mathbb{1}}.$$

A linear functional L on $\mathbb{M}_n \otimes \mathbb{M}_n$ is

(1) *real* if $L(M^*) = \overline{L(M)}$ for all $M \in \mathbb{M}_n \otimes \mathbb{M}_n$,
(2) *weakly positive* if $L(A \otimes B) \geqslant 0$ whenever $A \geqslant 0$ and $B \geqslant 0$,
(3) *positive* if $L(M) \geqslant 0$ for all positive $M \in \mathbb{M}_n \otimes \mathbb{M}_n$.

The following proposition may be derived from Equations (6) and (7) and Proposition 5.

PROPOSITION 6. *L_ϕ is positive (weakly positive, real) if and only if ϕ is completely positive (positive, hermitian).*

The content of Proposition 6 is contained in [10]. We confine ourselves to the following remarks.

REMARK 9. The representation (2) of the completely positive map ϕ corresponds by Proposition 5 to the decomposition of the positive linear functional L_ϕ into its extreme points. Since the state space $\mathbb{M}_n \otimes \mathbb{M}_n$ is not a simplex, this decomposition is not unique. Equivalently, we can consider the decomposition of the positive operator δL_ϕ into its spectral resolution. We then obtain the representation (2) where the $V^{(\alpha)}$ are orthogonal with respect to the Hilbert-Schmidt scalar product $\langle\ ,\ \rangle$.

REMARK 10. Equation (7) and Proposition 6 give a transparent proof of Choi's result [15] that an n-positive map of $\mathbb{M}_n$ is completely positive: If ϕ is n-positive, then $\hat{\phi}$ [Equation (7)] is positive and thus L_ϕ is positive. Hence ϕ is completely positive.

REMARK 11. The linear functional L on $\mathbb{M}_n \otimes \mathbb{M}_n$ is *doubly chaotic* if its restriction to each of the factors $\mathbb{M}_n$ is the totally chaotic state ω. From Propositions 4 and 6 and Remark 7, the correspondence (6) sets up a one-one correspondence between doubly stochastic completely positive maps of $\mathbb{M}_n$ and doubly chaotic states on $\mathbb{M}_n \otimes \mathbb{M}_n$.

5.2. *The Tilde Operation*

Let ϕ be a linear map of $\mathbb{M}_n$ into itself, and L_ϕ the corresponding linear functional on $\mathbb{M}_n \otimes \mathbb{M}_n$. Let $P_{\mathbb{1}} \in B(\mathbb{M}_n)$ be the projection onto $\mathbb{1} \in \mathbb{M}_n$ (Remark 8), and $P_{\mathbb{1}}^{\perp}$ the projection onto the orthogonal complement of $\mathbb{1}$.

We then have

$$\delta L_\phi = P_{\mathbb{1}}^{\perp}\ \delta L_\phi P_{\mathbb{1}}^{\perp} + P_{\mathbb{1}}\ \delta L_\phi P_{\mathbb{1}}^{\perp} + P_{\mathbb{1}}^{\perp}\ \delta L_\phi P_{\mathbb{1}} + P_{\mathbb{1}}\ \delta L_\phi P_{\mathbb{1}}$$

$$= \widetilde{\delta L}_\phi + \delta L_{\mathbb{1}, S} + \delta L_{S', \mathbb{1}}$$

where

$$\widetilde{\delta L}_\phi = P_{\mathbb{1}}^{\perp}\ \delta L_\phi P_{\mathbb{1}}^{\perp} \tag{8}$$

and

$$S = \delta L_\phi \mathbb{1} - \tfrac{1}{2}\langle \mathbb{1}, \delta_{L\phi}\mathbb{1}\rangle \mathbb{1},$$

$$S' = \delta L_\phi^* \mathbb{1} - \tfrac{1}{2}\langle \mathbb{1}, \delta_{L\phi}^*\mathbb{1}\rangle \mathbb{1},$$

where * denotes the adjoint on $B(\mathbb{M}_n)$. Correspondingly we obtain, from Proposition 5,

$$\phi = \tilde{\phi} + S'^* \cdot + \cdot S.$$

The tilde operation is defined by the transformation $\phi \to \tilde{\phi}$.

REMARK 12.

(i) If ϕ is hermitian, then L_ϕ is real and $\delta L_\phi^* = \delta L_\phi$. Hence $S' = S$.

(ii) If ϕ is completely positive, then L_ϕ and δL_ϕ are positive and so is $\delta L_{\tilde{\phi}}$. Thus $\tilde{\phi}$ is completely positive.

We may give an explicit formula for $\tilde{\phi}$ in terms of the representation (2), using $P_{\mathbb{1}}^{\perp} C = C - \langle \mathbb{1}, C\rangle \mathbb{1} = C - (1/n)\operatorname{Tr} C\,\mathbb{1}$.

PROPOSITION 7. *If ϕ is represented as in Equation* (2), *then*

$$\tilde{\phi} = \sum_{\alpha=1}^{a} \widetilde{V^{(\alpha)*}} \cdot \widetilde{V^{(\alpha)}},$$

where $\widetilde{V^{(\alpha)}} = V^{(\alpha)} - [(1/n)\operatorname{Tr} V^{(\alpha)}]\mathbb{1}$.

5.3. The Generator of a Completely Positive Semigroup

We observe that $\tilde{\phi}$ and S depend smoothly on ϕ, so that if $\phi(t)$ is a differentiable one-parameter family of linear maps, then $\widetilde{\phi(t)}$ and $S(t)$ are differentiable in t. Furthermore, since the identity map corresponds to $P_{\mathbb{1}}$, it follows that

$$\widetilde{\mathrm{Id}} = 0.$$

Thus

$$\left.\frac{d}{dt}\right|_{t=0} \widetilde{\phi(t)} = \lim_{t\to 0} \frac{1}{t}\widetilde{\phi(t)}.$$

We conclude from Remark 12

PROPOSITION 8. *If $\phi(t)$ is a differentiable family of completely positive maps, then*

$$\left.\frac{d}{dt}\right|_{t=0} \phi(t) = \mathscr{J} + \mathscr{K}$$

where $\mathscr{J} = \lim_{t\to 0}(1/t)\phi(t)$ is completely positive and

$$\mathscr{K} = T^* \cdot + \cdot T, \qquad T = \left.\frac{d}{dt}\right|_{t=0} S(t).$$

The converse follows easily from the Lie product formula, and we have thus obtained a transparent derivation of the general form of the generator of a completely positive semigroup [16–19]:

GORINI-KOSSAKOWSKI-LINDBLAD-SUDARSHAN THEOREM [16, 17]. *The map Γ generates a completely positive semigroup on $\mathbb{M}_n$ if and only if $\Gamma = \mathscr{J} + \mathscr{K}$ where $\mathscr{J}$ is completely positive and $\mathscr{K} = T^* \cdot + \cdot T$ for some $T \in \mathbb{M}_n$.*

Although formulated somewhat differently, the approach in [18] is essentially equivalent to the method used here.

PROPOSITION 9. *If $\phi(t) = \exp(t\Gamma)$, where $\Gamma = \mathscr{L} + \mathscr{K}$, $\mathscr{L}$ is arbitrary, and $\mathscr{K} = T^* \cdot + \cdot T$ for some $T \in \mathbb{M}_n$, then*

$$\mathscr{L} = \lim_{t\to 0} \frac{1}{t}\tilde{\phi}(t).$$

Proof.

$$\lim_{t\to 0} \frac{1}{t}\phi(t) = \frac{d}{dt}\bigg|_{t=0} \phi(t) = \tilde{\Gamma} = \tilde{\mathscr{L}},$$

since $\tilde{\mathscr{K}} = 0\ (P_{\mathbb{1}}^{\perp}\ \mathbb{1} = 0)$. ■

6. AN ELEMENTARY DERIVATION OF A RESULT OF KUMMERER AND MAASSEN

In this section we consider the class of examples constructed by Kummerer and Maassen [4], who constructed doubly stochastic completely positive semigroups which are not convex combinations of unitary maps. We shall give an elementary derivation of their result, based on the tilde technique, which does not rely on Hunt's theorem.

Let $\phi(t) = \exp(t\Gamma)$, $\Gamma = \mathscr{J} + T^* \cdot + \cdot T$, where $\mathscr{J}$ is completely positive and $T \in \mathbb{M}_n$. Then $\phi(t)$ is a continuous semigroup of completely positive maps. According to Proposition 9

$$\tilde{\mathscr{J}} = \lim_{t\to 0} \frac{1}{t}\phi(t). \tag{9}$$

Equation (9) is useful in relating properties of $\mathscr{J}$ to properties of $\phi(t)$, in particular the property that $\phi(t)$ is a convex combination of unitary maps.

Express $\phi(t)$ according to the representation (2) with a fixed. Equation (9) and Proposition 7 give

$$\tilde{\mathscr{J}} = \lim_{t\to 0} \sum_{\alpha=1}^{a} W^{(\alpha)}(t)^* \cdot W^{(\alpha)}(t), \tag{10}$$

where $W^{(\alpha)}(t) = (1/\sqrt{t}\,)V^{(\alpha)}(t)$.

PROPOSITION 10. *There exists a sequence $t_k \to 0$ such that for each α,*

$$W^{(\alpha)}(t_k) \to Z^{(\alpha)} \quad \text{and} \quad \tilde{\mathscr{J}} = \sum_{\alpha=1}^{a} Z^{(\alpha)*} \cdot Z^{(\alpha)}.$$

Proof. From Equation (10), $\tilde{\mathscr{J}}(\mathbb{1}) = \lim_{t\to 0}\sum_{\alpha=1}^{a} W^{(\alpha)}(t)^* W^{(\alpha)}(t)$. It follows by a compactness argument that a sequent $t_k \to 0$ exists such that $W^{(\alpha)}(t_k)$ converges for each α. ■

Following Kummerer and Maassen [4], let $\mathscr{J} = A^* \cdot A$, where A is normal, and let $T = -\frac{1}{2}A^*A + iH$, where $H = H^*$ is arbitrary. Then $\phi(t)$ is a doubly stochastic completely positive semigroup.

KUMMERER AND MAASSEN'S THEOREM [4, Proposition 2.2.1]. *If the spectrum of A does not lie on a circle or on a line, then $\phi(t)$ is not a convex combination of unitary maps for each t.*

Proof. Assume that for each $t \geqslant 0$, $\phi(t)$ is a convex combination of unitary maps. Then we may express $\phi(t)$ as in the representation (2) with each $V^{(\alpha)}(t)$ a multiple of a unitary matrix. (By Carathéodory's theorem [20, Theorem 18] we may take a fixed.) Since $\tilde{\mathscr{J}} = \tilde{\mathscr{A}}^* \cdot \tilde{A}$ and $\tilde{\mathscr{J}}$ is expressed as in Proposition 10, it follows that each $Z^{(\alpha)}$ is a multiple of $\tilde{A}$. Since the spectrum of $V^{(\alpha)}$ lies on a circle and therefore the spectrum of $W^{(\alpha)}$ lies on a circle, it follows that the spectrum of $Z^{(\alpha)}$ either lies on a circle or on a limit of a circle, namely a straight line. The same then holds for $\tilde{A}$ and for A. ∎

REMARK 13. In the above construction A is normal and therefore may be diagonalized by a unitary matrix. The constructed semigroup above is therefore unitarily equivalent to a diagonal semigroup (if H commutes with A). According to the discussion in Section 4, $n = 4$ is the smallest value of n such that diagonal maps of $\mathbb{M}_n$ may not be convex combinations of unitary maps. Notice that n complex numbers always lie on a circle or a line if $n < 4$.

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