

## A PROBLEM RELATING TO POSITIVE LINEAR MAPS ON MATRIX ALGEBRAS

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In this paper we investigate conditions under which two finite-dimensional density matrices can be transformed simultaneously into two other ones by means of a positive linear map which maps density matrices into density matrices. The result of this paper provides a complete answer in case of the matrix algebra of two-by-two matrices.

### 1. The problem

Let  $M_n$  denote the  $C^*$ -algebra of complex  $n \times n$ -matrices. By  $\text{Tr}(\cdot)$  we mean the standard trace on  $M_n$ . Whenever  $A \in M_n$  by  $\|A\|_1$  we mean the  $L_1$ -norm (functional norm) of the element  $A$ , i.e.  $\|A\|_1 = \sup_{\|C\| \leq 1} |\text{Tr} AC|$ , where  $\|\cdot\|$  indicates the  $C^*$ -norm on  $M_n$ .

DEFINITION (stochastic maps). A linear transformation  $L$  acting from  $M_n$  into  $M_n$  is said to be *stochastic* if  $L$  maps the positive cone of  $M_n$  into itself and  $\text{Tr} L(A) = \text{Tr} A$  for all  $A \in M_n$ .

As usually, a density matrix of  $M_n$  is understood to be a non-negative matrix with trace equal to one. Thus, stochastic mappings are exactly those linear maps on  $M_n$  which carry density matrices into density matrices. In this paper we shall deal with a particular case of the following problem concerning density matrices and stochastic transformations:

Give necessary and sufficient conditions under which a given (but arbitrarily chosen) pair  $(Z, Z')$  of density matrices can be transformed into another given (but arbitrarily chosen) pair  $(X, Y)$  by means of a stochastic map.

We will give a solution of the problem in the case of the matrix algebra  $M_2$ . We state our result in the following

**THEOREM.** *Let  $X, Y, Z, Z'$  be density matrices from  $M_2$ . Then there exists a stochastic map  $L$  on  $M_2$  such that*

$$X = \mathbf{L}(Z) \quad \text{and} \quad Y = \mathbf{L}(Z') \quad (1)$$

if and only if

$$\|X - tY\|_1 \leq \|Z - tZ'\|_1 \quad \text{for all } t \in \mathbf{R}_+^1 \quad (2)$$

( $\mathbf{R}^1$  denotes the real axis). Moreover, whenever (2) holds a completely positive stochastic  $\mathbf{L}$  satisfying (1) can be chosen.

We note that the implication (1)  $\rightarrow$  (2) is almost trivial, for any stochastic map is  $L_1$ -contracting. Thus, in the proof we will have to show validity of the implication (2)  $\rightarrow$  (1) for a completely positive stochastic ( $CP$ -stochastic)  $\mathbf{L}$ .

We conclude this introductory part with some remarks. Although two-by-two matrices show some specific properties which allow to solve exemplarily basic problems relating to the structure of convex sets of completely positive and positive linear maps over  $M_2$  (cf. [2], [9], and [11]), we believe that our problem is more closely related to  $CP$ -stochasticity than to general stochasticity in the general case, too. In fact, conditions like (2) on  $M_n$  are strong enough to guarantee the existence of a  $CP$ -map transforming one pair of density matrices into another one. The difficulties arise from the requirement that our maps have to be stochastic ones! Furthermore, in some special cases necessary and sufficient conditions are known. Thus, in case  $Y = Z' = \frac{1}{n}\mathbf{1}$  ( $\mathbf{1}$

denoting the unit matrix in  $M_n$ ) the conditions  $\|X - t\mathbf{1}\|_1 \leq \|Z - t\mathbf{1}\|_1$  for all non-negative reals are necessary and sufficient. Here, proofs using the  $e_s$ -number approach in context with the order structure of states are known (cf. [1], [10]).

Moreover, in case  $XY = YX$  and  $ZZ' = Z'Z$  a consequence of the result obtained in [5] in employing classical statements proved in [4] and [7] is that  $\|X - tY\|_1 \leq \|Z - tZ'\|_1$  for all  $t \in \mathbf{R}_+^1$  is the decisive condition. In using the well-known extension theorem for  $CP$ -maps (see [2]) these results may be traced over to more general cases, e.g. type  $\text{II}_1$  factors.

There are also some results relating to the general problem for  $M_n$  with  $n > 2$ . Here by examples one is assured of the fact that the condition  $\|X - tY\|_1 \leq \|Z - tZ'\|_1 \quad \forall t \in \mathbf{R}_+^1$  is not sufficient. It has to be replaced by a more complex condition closely related to complete positivity. We will comment on this a forthcoming paper.

## 2. Notations

In this part we introduce some notations and conventions to be used throughout the following parts. For convenience we will work in  $M_2 \times M_2$  equipped with the usual topology. We start with

DEFINITION 1. (*K*-sets) Let  $Z, Z'$  be density matrices in  $M_2$ . We set

$$K(Z, Z') = \{(X, Y) \in M_2 \times M_2 : \|X - tY\|_1 \leq \|Z - tZ'\|_1 \text{ for all } t \geq 0, X, Y \text{ - density matrices}\}; \tag{1}$$

$$K_0(Z, Z') = \{(X, Y) \in M_2 \times M_2 : \text{there exists a CP-stochastic map } L \text{ on } M_2 \text{ with } (X, Y) = (L(Z), (L(Z')))\}. \tag{2}$$

Note that both sets introduced in Definition 1 are convex and compact (in  $M_2 \times M_2$ ).

DEFINITION 2. (*s*-numbers) Let  $X, Y$  be density matrices in  $M_2$ . We define

$$s_1(X, Y) = \sup_{X - tY \geq 0} t \tag{3}$$

$$s_2(X, Y) = \begin{cases} \inf_{X - tY \leq 0} t & \text{in case } (X - tY)_+ = 0 \text{ for a } t \geq 0, \\ +\infty & \text{if } (X - tY)_+ \neq 0 \text{ for all } t \geq 0, \end{cases} \tag{4}$$

where  $A_+$  is the positive part of  $A$  in  $M_2$ .

Since  $X, Y$  are density matrices we have

$$0 \leq s_1(X, Y) \leq 1 \leq s_2(X, Y) \leq +\infty. \tag{5}$$

Now we state some useful and obvious implications: Let  $X, Y, Z, Z'$  be density matrices.

$$\text{If } 0 < s_1(X, Y) < 1 < s_2(X, Y) < +\infty \text{ then } X, Y \text{ are invertible.} \tag{6}$$

$$\text{If } 0 = s_1(X, Y) \text{ then } X \text{ is an orthoprojection.} \tag{7}$$

$$\text{If } +\infty = s_2(X, Y) \text{ then } Y \text{ is an orthoprojection.} \tag{8}$$

$$\text{If } s_1(X, Y) = 1 \text{ then } X = Y. \tag{9}$$

$$\text{If } s_2(X, Y) = 1 \text{ then } X = Y. \tag{10}$$

$$(X, Y) \in K(Z, Z') \text{ iff } \|(X - tY)_+\|_1 \leq \|(Z - tZ')_+\|_1 \forall t \geq 0. \tag{11}$$

The latter follows from the fact that  $\|X - tY\|_1 + (1 - t) = 2\|(X - tY)_+\|_1$  for all  $t$ . The expression  $\|(X - tY)_+\|_1$  will play an important role in all subsequent argumentations.

As a function of  $t$   $\|(X - tY)_+\|_1$  has some useful properties:

$$\|(X - tY)_+\|_1 \text{ is convex, continuous and decreasing on the reals;} \tag{12}$$

$$\|(X - tY)_+\|_1 \geq 1 - t \text{ for all reals } t, \tag{13}$$

$$\|(X - tY)_+\|_1 = 1 - t \quad \text{for } t \leq s_1(X, Y), \tag{14}$$

$$\|(X - tY)_+\|_1 = 0 \quad \text{for } t \geq s_2(X, Y) \text{ (in case } s_2(X, Y) < \infty), \tag{15}$$

$$\|(X - tY)_+\|_1 > \max\{0, 1 - t\} \quad \text{if } s_1(X, Y) \neq 1 \tag{16}$$

for all  $t$  with  $s_1(X, Y) < t < s_2(X, Y)$ .

To conclude this part we prove three results about  $s$ -numbers and  $K$ -sets.

LEMMA 1. *Let  $X, Y, Z, Z'$  be density matrices in  $M_2$ . Then,  $(X, Y) \in K(Z, Z')$  implies*

$$0 \leq s_1(Z, Z') \leq s_1(X, Y) \leq s_2(X, Y) \leq s_2(Z, Z'). \tag{17}$$

*Proof:* Assume  $s_1(Z, Z') = 1$ . Then  $Z = Z'$  by (9). From (11) then follows that  $\|(X - Y)_+\|_1 = 0$ , so  $\|X - Y\|_1 = 0$  by the relation  $\|X - Y\|_1 = 2\|(X - Y)_+\|_1$ , i.e.  $X = Y$ . This implies the equality  $s_1(X, Y) = 1 = s_2(X, Y)$  which proves our statement in case  $Z = Z'$ .

Assume  $Z \neq Z'$ . Then,  $s_1(Z, Z') < 1 < s_2(Z, Z')$ . Suppose  $s_1(X, Y) < s_1(Z, Z')$ . Since  $(X, Y) \in K(Z, Z')$ , we have  $\|(X - tY)_+\|_1 \leq \|(Z - tZ')_+\|_1 = 1 - t$  for all  $t$  satisfying  $s_1(X, Y) \leq t \leq s_1(Z, Z') < 1$ . This contradicts (16). Hence  $s_1(Z, Z') \leq s_1(X, Y)$  holds necessarily.

Assume  $s_2(Z, Z') = +\infty$ . Then obviously  $s_2(X, Y) \leq s_2(Z, Z')$ . Let  $s_2(Z, Z') < +\infty$ . Since  $(X, Y) \in K(Z, Z')$ , we have  $s_2(X, Y) < +\infty$  and because of  $\|(X - tY)_+\|_1 \leq \|(Z - tZ')_+\|_1$  for all  $t \geq 0$  we have for  $t = s_2(Z, Z') = s_2$  the relation  $\|(X - s_2Y)_+\|_1 = 0$ , i.e.  $(X - s_2Y)_+ = 0$ , so  $s_2 = s_2(Z, Z') \geq s_2(X, Y)$  by definition of  $s$ -numbers. q.e.d.

LEMMA 2. *Let  $X, Y, Z, Z'$  be density matrices in  $M_2$ . Assume that  $s_1(Z, Z') \leq s_1(X, Y) \leq s_2(Z, Z')$  holds. Then  $(X, Y) \in K(Z, Z')$  iff*

$$\|(X - tY)_+\|_1 \leq \|(Z - tZ')_+\|_1 \tag{18}$$

for all  $t$  in the interval  $s_1(X, Y) \leq t \leq s_2(X, Y)$ .

*Proof:* Necessity is obvious. Assume (18) to hold for  $s_1(X, Y) \leq t \leq s_2(X, Y)$ . Then from the definition of  $s_2$ -number and (15) it follows that (18) also holds for  $t \geq s_2(X, Y)$ . By (14) we see that (18) is valid for  $t \leq s_1(Z, Z')$ . Finally we use (13) and (14) to prove validity of (18) for  $s_1(Z, Z') \leq t \leq s_1(X, Y)$ . Thus, (18) is valid for any non-negative real. Then from (11) it follows that  $(X, Y) \in K(Z, Z')$ . q.e.d.

LEMMA 3. *Let  $X, Y, Z, Z'$  be density matrices in  $M_2$ . Then  $(X, Y) \in K(Z, Z')$  if and only if*

$$s_1(Z, Z') \leq s_1(X, Y) \leq s_2(X, Y) \leq s_2(Z, Z'), \tag{19}$$

and

$$\text{Det}(X - tY) \geq \text{Det}(Z - tZ') \tag{20}$$

for all  $t$  in the interval  $s_1(X, Y) \leq t \leq s_2(X, Y)$ .

*Proof:* From Lemma 1 we see (19) is necessary for  $(X, Y) \in K(Z, Z')$ . We compute  $\|(X - tY)_+\|_1, \|(Z - tZ')_+\|_1$  for all  $t$  in the interval in question under the condition that (19) is valid. By definition of  $s$ -number we have

$$\|(X - tY)_+\|_1 = \text{the non-negative eigenvalue of } (X - tY), \tag{21}$$

$$\|(Z - tZ')_+\|_1 = \text{the non-negative eigenvalue of } (Z - tZ'). \tag{22}$$

(21) and (22) are the non-negative solutions of

$$\lambda^2 - (1 - t)\lambda + \text{Det}(X - tY) = 0 \tag{23}$$

and

$$\lambda^2 - (1 - t)\lambda + \text{Det}(Z - tZ') = 0, \text{ respectively.} \tag{24}$$

The non-negative solution of (23) for all  $t$  from the interval  $s_1(X, Y) \leq t \leq s_2(X, Y)$  is

$$\lambda_+ = (1 - t)/2 + [(1 - t)^2/4 - \text{Det}(X - tY)]^{1/2}. \tag{25}$$

Thus, under the condition that (19) holds, we infer from (25) and the corresponding solution of (24) that (20) implies  $\|(X - tY)_+\|_1 \leq \|(Z - tZ')_+\|_1$  for  $t \in [s_1(X, Y), s_2(X, Y)]$ . Taking into account Lemma 2 we get  $(X, Y) \in K(Z, Z')$ . Thus, (19) and (20) are sufficient conditions. Necessity of (19), (20) follows from Lemma 1 and (25) together with the non-negative solution of (24). q.e.d.

### 3. Some special cases

In this part we discuss some cases that play a decisive role in the general proof of our theorem. We start with

LEMMA 1. *Let  $X, Z, Z'$  be density matrices in  $M_2$ . Then  $(X, X) \in K_0(Z, Z')$ .*

*Proof:* Let  $U$  be a unitary matrix diagonalizing  $X$ , i.e.  $UXU^* = \begin{bmatrix} x & 0 \\ 0 & 1-x \end{bmatrix}$ , where  $0 \leq x \leq 1$ . We define the matrices  $\{A_i\}_{i=1}^4$  by

$$\begin{aligned} A_1 &= x^{1/2} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, & A_2 &= x^{1/2} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \\ A_3 &= (1-x)^{1/2} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, & A_4 &= (1-x)^{1/2} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \end{aligned} \tag{1}$$

Then an easy check shows that

$$P = \sum_i U^* A_i(\cdot) A_i^* U \tag{2}$$

is stochastic and defines a CP-map with  $X = P(Z) = P(Z')$ . q.e.d.

Now we state the first particular case of our theorem:

LEMMA 2. *Let  $X$  be a density matrix in  $M_2$ . Then  $K(X, X) = K_0(X, X)$ .*

*Proof:* By our remark after the Theorem in 1, we can be sure that  $K_0(X, X) \subset K(X, X)$ . Now, assume  $(Z, Z') \in K(X, X)$ . Then by the definition of  $K(X, X)$  we have  $\|Z - Z'\|_1 \leq 0$ , thus  $Z = Z'$ . By Lemma 1 we see  $(Z, Z') = (Z, Z) \in K_0(X, X)$ , i.e.  $K(X, X) \subset K_0(X, X)$ . Hence  $K_0(X, X) = K(X, X)$ . q.e.d.

Whereas the preceding results are of more or less trivial character, the following requires more attention.

LEMMA 3. *Let  $X, Y$  be density matrices in  $M_2$  and  $P, Q$  one-dimensional orthoprojections in  $M_2$ . Then whenever  $(Y, P) \in K(X, Q)$  (resp.  $(P, Y) \in K(Q, X)$ ) we find that  $(Y, P) \in K_0(X, Q)$  (resp.  $(P, Y) \in K_0(Q, X)$ ).*

*Proof:* Since  $\|T - tT'\|_1 = t\|T' - t^{-1}T\|_1$  for all  $t > 0$  the validity of the implication  $(P, Y) \in K(Q, X) \rightarrow (P, Y) \in K_0(Q, X)$  follows from  $(Y, P) \in K(X, Q) \rightarrow (Y, P) \in K_0(X, Q)$ . We prove the latter. Assume for the moment that this has been shown, i.e. we have CP-stochastic  $L$  transforming the pair  $(X, Q)$  into  $(Y, P)$ . Let  $U$  be a unitary matrix transforming  $P$  into  $Q$ , i.e.  $UPU^* = Q$ . Then we have  $(UYU^*, Q) = (P(X), P(Q))$  with  $P = U L(\cdot) U^*$ , and  $P$  is CP-stochastic. Since  $U$  is unitary and  $K(X, Q)$  is unitary invariant, our problem is equivalent to that of proving the implication  $(A, Q) \in K(B, Q) \rightarrow (A, Q) \in K_0(B, Q)$ . By analogous argumentation we may suppose  $Q$  to be of the form  $Q = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ . Since for a CP-stochastic  $L$  the mapping  $P = U L(V \cdot V^*) U^*$  is CP-stochastic whenever  $U, V$  are unitaries, we may consider our problem reduced to the case when

$$A = \begin{bmatrix} a & \delta\sqrt{a(1-a)} \\ \delta\sqrt{a(1-a)} & 1-a \end{bmatrix}, \quad B = \begin{bmatrix} b & \sqrt{b(1-b)} \\ \varepsilon\sqrt{b(1-b)} & 1-b \end{bmatrix},$$

where  $0 \leq a, b \leq 1$ ,

$0 \leq \delta, \varepsilon \leq 1$ . This common choice of real (positive) phase is possible by taking for  $U, V$  unitaries of the form  $\begin{bmatrix} 1 & 0 \\ 0 & e^{i\beta} \end{bmatrix}$  with appropriate real  $\beta$ 's. Since these unitaries commute with  $Q = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ , all we have to prove is that

$$(A, Q) \in K(B, Q) \quad \text{implies} \quad (A, Q) \in K_0(B, Q), \tag{3}$$

where

$$Q = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad A = \begin{bmatrix} a & \delta\sqrt{a(1-a)} \\ \delta\sqrt{a(1-a)} & 1-a \end{bmatrix}, \quad B = \begin{bmatrix} b & \varepsilon\sqrt{b(1-b)} \\ \varepsilon\sqrt{b(1-b)} & 1-b \end{bmatrix}, \tag{4}$$

with

$$0 \leq a, b \leq 1, \quad 0 \leq \delta, \varepsilon \leq 1. \tag{5}$$

By virtue of Lemma 1, Lemma 2 we can reduce our problem to the one where (5) is replaced by

$$0 \leq b < 1, \quad 0 < a \leq 1; \quad \text{if } a = b, \text{ so } \varepsilon \neq 0. \tag{6}$$

We shall verify that (6) is the non-trivial part of (5). First, suppose  $b = 1$ . Then Lemma 1 is applicable and (3) holds. Secondly, suppose  $a = 0$ , i.e.  $A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ . This implies

$\|(A - tQ)_+\|_1 = \left\| \left[ \begin{array}{cc} -t & 0 \\ 0 & 1 \end{array} \right]_+ \right\|_1 = 1$  for all  $t \geq 0$ . Thus  $\|(B - tQ)_+\|_1 = 1$  (since 1 is the maximum value of  $\|(X - tY)_+\|_1$  for density matrices  $X, Y$  and  $t \geq 0$ . The latter occurs iff  $BQ = 0$  (as can be easily verified). Thus,  $A = B$  must be required (since we are working with two-by-two matrices). But then  $(A, Q) \in K_0(B, Q)$  is trivial (take  $L =$  identity map). Thirdly, let be  $a = b, \varepsilon = 0$ . Since  $(A, Q) \in K(B, Q)$  is assumed, we have

$$\left\| \left[ \begin{array}{cc} a - t & \delta\sqrt{a(1-a)} \\ \delta\sqrt{a(1-a)} & 1 - a \end{array} \right] \right\|_1 \leq \left\| \left[ \begin{array}{cc} a - t & 0 \\ 0 & 1 - a \end{array} \right] \right\|_1 \quad \text{for all } t \geq 0.$$

By 2, Lemma 1 this requires  $s_1(A, Q) \geq s_1(B, Q) = a$ . Then, in particular for  $t = a, A - aQ \geq 0$  must hold. With  $a \neq 0, 1$  this is only possible if  $\delta = 0$ , i.e.  $A = B$  and the identity map can be chosen to carry the pairs into each other. The case  $a = 0$  (resp.  $a = 1$ ) is discussed in the second (resp. first) possibility. Our discussions show that (6) is the non-trivial part of (5). We have to prove (3) under the conditions (4) and (6). We start with deriving necessary conditions for  $(A, Q) \in K(B, Q)$ , i.e. we may suppose that

$$\|(A - tQ)_+\|_1 \leq \|(B - tQ)_+\|_1 \quad \text{for all } t \geq 0 \tag{7}$$

holds (see 2 (11)). The latter, however, means for sufficiently large  $t$  that

$$\text{Det}(A - tQ) \geq \text{Det}(B - tQ) \quad (\text{cf. 2, Lemma 3}). \tag{8}$$

We write down (8) in explicit form

$$(a - t)(1 - a) - \delta^2 a(1 - a) \geq (b - t)(1 - b) - \varepsilon^2 b(1 - b). \tag{9}$$

(9) means that

$$\text{Det } A - \text{Det } B \geq t(b - a) \tag{10}$$

for all  $t$  taken from  $s_1(A, Q) \leq t \leq s_2(A, Q)$  (cf. 2, Lemma 3). Excluding the trivial case  $A = Q$  (i.e.  $a = 1$ ) in (6) which implies that (3) is valid by Lemma 1, we see that

$$\text{for } a \neq 1 \quad \text{we have} \quad s_2(A, Q) = +\infty. \tag{11}$$

Therefore, in this case from (10) follows that

$$b \leq a, \quad (12)$$

where we used (11).

In particular, for  $t = s = s_1(A, Q)$  we find from the definition of  $s_1$  that

$$(b - s)(1 - b) \leq \varepsilon^2 b(1 - b), \quad (a - s)(1 - a) = \delta^2 a(1 - a). \quad (13)$$

In deriving (13) we had to take into account 2, Lemma 1. From (13) we get

$$(1 - \delta^2)a = s \geq (1 - \varepsilon^2)b, \quad (14)$$

where we made use of (6) and excluded the trivial case  $a = 1$ . (14) implies that

$$\delta^2 \leq 1 - (1 - \varepsilon^2)(b/a) \quad (15)$$

by (6) again. This means by (6) and (12) that

$$\delta \leq [1 - (1 - \varepsilon^2)(b/a)]^{1/2}. \quad (16)$$

Consider the following matrices

$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & \alpha \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & \omega \\ 0 & \beta \end{bmatrix}, \quad A_3 = \begin{bmatrix} 0 & 0 \\ 0 & \gamma \end{bmatrix}, \quad (17)$$

where

$$\alpha = \left( \frac{b(1-a)}{a(1-b)} \right)^{1/2} \frac{\varepsilon\delta}{1 - (1 - \varepsilon^2)(b/a)}. \quad (18)$$

$$\beta = \left( \frac{(a-b)(1-a)}{(1-b)a} \right)^{1/2} \frac{\delta}{1 - (1 - \varepsilon^2)(b/a)}, \quad (19)$$

$$\gamma = \left( \frac{(1 - \delta^2) - (1 - \varepsilon^2)(b/a)}{1 - (1 - \varepsilon^2)(b/a)} \right)^{1/2} \left( \frac{1-a}{1-b} \right)^{1/2}, \quad (20)$$

$$\omega = \left( \frac{a-b}{1-b} \right)^{1/2}, \quad (21)$$

and by (6) and (16) and (12) these values are well-defined reals. We define a CP-map by

$$L = A_1(\cdot)A_1^* + A_2(\cdot)A_2^* + A_3(\cdot)A_3^*. \quad (22)$$

Then by direct computations (which we omit) one shows that  $L$  is trace-preserving and

$$L(Q) = Q, \quad L(B) = A. \quad (23)$$



Since (23) remains valid for  $a = 1$ , the implication (3) is seen to hold under (6), and therefore, as a consequence of our discussions, under condition (5). This completes the proof. q.e.d.

**4. The final proof**

We have to prove that  $K(Z, Z') = K_0(Z, Z')$  for any density matrices  $Z, Z'$ , because of 3, Lemma 2 we may restrict our proof on the case  $Z \neq Z'$ . Let  $\text{ex } K(Z, Z')$  denote the set of extreme points of  $K(Z, Z')$ . Since  $K(Z, Z')$  is compact,  $K(Z, Z')$  is the closure of the convex hull of  $\text{ex } K(Z, Z')$ . We begin with a result on the extreme points:

STATEMENT 1. *Let  $X, Y, Z, Z'$  be density matrices of  $M_2$  with  $Z \neq Z'$ . Assume  $(X, Y) \in K(Z, Z')$  with*

$$s_1(Z, Z') < s_1(X, Y) < s_2(X, Y) < s_2(Z, Z'). \tag{1}$$

*Then,  $(X, Y) \notin \text{ex } K(Z, Z')$ .*

For the proof we need

LEMMA 1. *Let  $X, Y, Z, Z'$  be as in the assumption of Statement 1. Then there exists at most one value  $t_0$  with  $s_1(X, Y) \leq t_0 \leq s_2(X, Y)$  such that*

$$\text{Det}(X - t_0 Y) = \text{Det}(Z - t_0 Z'). \tag{2}$$

*Moreover, if (2) occurs at  $t_0$  from the interval in question, then*

$$s_1(X, Y) < t_0 < s_2(X, Y). \tag{3}$$

*Proof of Lemma 1:* We define a function  $D(t)$  on  $\mathbb{R}^1$  by

$$D(t) = \text{Det}(X - tY) - \text{Det}(Z - tZ'). \tag{4}$$

Then our assumptions together with 2, Lemma 3 and 2, (13), (14) imply

$$D(t) \geq 0 \quad \text{for all } t \text{ from } s_1(X, Y) \leq t \leq s_2(X, Y) \tag{5}$$

and at the endpoints of the interval

$$D(s_1(X, Y)) > 0, \quad D(s_2(X, Y)) > 0. \tag{6}$$

Thus, whenever (2) holds for  $t_0$  from the interval in question we will find  $t_0$  in the interior due to (6).

Now, the equation  $D(t) = 0$  is of (at most) second degree in  $t$ . Hence, there exist at most two real solutions (because of (6)  $D(t)$  cannot be equal to zero). Suppose there is one solution – say  $t_0$  – in  $s_1(X, Y) < t_0 < s_2(X, Y)$  (cf. (3)). Then for the derivative  $D'(t)$  of  $D(t)$  we find

$$D'(t_0) = 0. \tag{7}$$

In fact, for  $D'(t_0) > 0$  we had  $D'(t) > 0$  in a neighbourhood of  $t_0$ , i.e. by (5) we had  $D(t_0) > 0$ , a contradiction. In case  $D'(t_0) < 0$  we had  $D'(t) < 0$  for all  $t > t_0$  sufficiently close to  $t_0$ , so  $D(t) < 0$  there, a contradiction to (5). This proves (7). Since  $D'(t)$  is a linear function of  $t$ ,  $D'(t)$  is monotonous. Then (7), (5) and (6) together with monotony imply that

$$D'(t) = \beta(t - t_0), \quad \text{with } \beta > 0. \tag{8}$$

Since  $D(t_0) = 0$ , (8) requires for  $D(t)$

$$D(t) = \frac{\beta}{2}(t - t_0)^2, \quad \text{with } \beta > 0. \tag{9}$$

The latter means that  $t_0$  is the only solution of  $D(t) = 0$  in  $s_1(X, Y) \leq t \leq s_2(X, Y)$  (cf. (6)). This proves Lemma 1. Moreover, we see from (8) that the existence of a solution of  $D(t) = 0$  in the interval in question automatically implies that this solution is a *double* root. q.e.d.

*Proof of Statement 1:* As mentioned several times before, in case of two-by-two matrices we may assume that

$$X^T = X, \quad Y^T = Y \quad ((\cdot)^T - \text{“transposition”}) \tag{10}$$

since this form can always be obtained by an appropriate unitary transformation. Let us define families of hermitian matrices:

$$a(r) = r \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}, \quad b(r) = t_0^{-1} a(r) \quad \text{for real } r, \tag{11}$$

where we suppose that  $t_0 \in (s_1(X, Y), s_2(X, Y))$ , with

$$D(t_0) = 0 \tag{12}$$

in case (2) occurs (so, in this case  $t_0$  is uniquely determined), and  $t_0$  is taken arbitrarily from the open interval in question if  $D(t) = 0$  has no root there. By means of (11) we define

$$X(r) = X + a(r), \quad Y(r) = Y + b(r), \tag{13}$$

and denote by  $D_r(t)$  the expression

$$D_r(t) = \text{Det}(X(r) - tY(r)) - \text{Det}(Z - tZ'). \tag{14}$$

Taking into account (10) one sees that

$$\begin{aligned} \text{Det}(X(r) - tY(r)) &= \text{Det}((X - tY) + (1 - t/t_0)a(r)) \\ &= \text{Det}(X - tY) - r^2(1 - t/t_0)^2. \end{aligned} \tag{15}$$

Therefore, (14) reads

$$D_r(t) = D(t) - r^2(1 - t/t_0)^2. \tag{16}$$

Now, two cases are possible:

I.  $D(t) > 0$  for all  $t$  with  $s_1(X, Y) \leq t \leq s_2(X, Y)$ . Then, because of (6) and due to (16) – and since  $s_1(X, Y)$  and  $s_2(X, Y)$  (the latter being  $< +\infty$ ) depend continuously on  $X, Y$  – we find  $k > 0$  such that

$$s_1(Z, Z') < s_1(X(\pm k), Y(\pm k)) < s_2(X(\pm k), Y(\pm k)) < s_2(Z, Z'), \tag{17}$$

and  $D_{\pm k}(t) > 0$  for all  $t$  taken from the correspondingly inner intervals. Moreover, since  $0 < s_1(X, Y) < 1 < s_2(X, Y) < +\infty$  both  $X, Y$  are invertible (cf. 2 (6)), so we can choose  $k$  such that  $X(\pm k), Y(\pm k)$  are density matrices (we notice that  $\text{Tr } a(r) = 0$ ).

Then by 2, Lemma 3 we see that

$$(X(\pm k), Y(\pm k)) \in K(Z, Z'), \tag{18}$$

i.e.  $(X, Y) = \frac{1}{2}(X(k), Y(k)) + \frac{1}{2}(X(-k), Y(-k))$  so since  $k \neq 0$ , therefore

$$(X, Y) \notin \text{ex } K(Z, Z') \tag{19}$$

II.  $D(t_0) = 0$  with  $s_1(X, Y) < t_0 < s_2(X, Y)$  (cf. Lemma 1). By (9) we then know that  $t_0$  is a *double* root of  $D(t) = 0$ . (9) and (16) together guarantee that  $t_0$  remains a *double* root of  $D_k(t) = 0$  for any sufficiently small  $k$ . Again we can stress the continuity argument in order to show the existence of  $k > 0$  such that

$$X(\pm k) \text{ and } Y(\pm k) \text{ are density matrices,} \tag{20}$$

$$s_1(Z, Z') < s_1(X(\pm k), Y(\pm k)) = s_1^\pm < t_0 < s_2^\pm = s_2(X(\pm k), Y(\pm k)) < s_2(Z, Z'). \tag{21}$$

$$D_{\pm k}(s_2^\pm) > 0, \quad D_{\pm k}(s_1^\pm) > 0. \tag{22}$$

Since  $D_{\pm k}(t) = 0$  is an equation of second degree with a double root and (22) holds, we are sure that  $D_{\pm k}(t)$  cannot change its sign in  $[s_1^\pm, s_2^\pm]$ , i.e. it has to be non-negative there. Again using 2, Lemma 3 and arguing exactly as at the end of Case I we infer that  $(X, Y) \notin \text{ex } K(Z, Z')$  in this case, too. Since all possibilities are exhausted by I and II, our statement is proven.

STATEMENT 2. *Let  $X, Y, Z, Z'$  be density matrices in  $M_2$ , with  $Z \neq Z'$ . Assume we have*

$$(X, Y) \in \text{ex } K(Z, Z'). \tag{23}$$

*Then,  $(X, Y)$  obeys one of the following conditions:*

$$s_1(Z, Z') = s_1(X, Y), \tag{24}$$

$$s_2(Z, Z') = s_2(X, Y), \quad (25)$$

$$s_1(X, Y) = 1. \quad (26)$$

*Proof:* A detailed proof can be omitted since the result is an obvious consequence of Statement 1.

LEMMA 2. Let  $X, Y, Z, Z'$  be density matrices in  $M_2$ , with  $Z \neq Z'$ . We assume

$$(X, Y) \in \text{ex}K(Z, Z'). \quad (27)$$

Then

$$(X, Y) \in K_0(Z, Z'). \quad (28)$$

*Proof:* Because of (27) Statement 2 becomes applicable. First assume

$$s_1(Z, Z') = s_1(X, Y) = s_1. \quad (29)$$

Then by the definition of  $s_1$  and (29) we have

$$Z - s_1 Z' = (1 - s_1)P, \quad X - s_1 Y = (1 - s_1)Q, \quad (30)$$

where  $P, Q$  are one-dimensional orthoprojections. From the condition  $(X, Y) \in K(Z, Z')$  and (30) it follows that

$$(1 - s_1) \|Q - t(1 - s_1)^{-1}Y\|_1 \leq (1 - s_1) \|P - t(1 - s_1)^{-1}Z'\|_1 \quad (31)$$

for all  $t \geq 0$  due to  $s_1 < 1$  which follows from  $Z \neq Z'$ , i.e.

$$(Q, Y) \in K(P, Z'). \quad (32)$$

From (32), however, together with 3, Lemma 3 follows

$$(Q, Y) \in K_0(P, Z'), \quad (33)$$

i.e. for a certain CP-stochastic  $L$

$$Q = L(P), \quad Y = L(Z'). \quad (34)$$

Together with (30), (34) shows that

$$X - L(s_1 Z') = L((1 - s_1)P), \quad \text{i.e.} \quad X = L(Z), \quad (35)$$

and therefore

$$(X, Y) = (L(Z), L(Z')), \quad \text{i.e.} \quad (X, Y) \in K_0(Z, Z'). \quad (36)$$

This proves (28) in case (29).

Secondly, suppose (27) holds with

$$s_2(Z, Z') = s_2(X, Y) = s_2 < +\infty. \quad (37)$$

By the definition of  $s_2$  we have then

$$Z - s_2 Z' = (1 - s_2)P, \quad X - s_2 Y = (1 - s_2)Q, \tag{38}$$

with one dimensional orthoprojections  $P, Q$ , and  $s_2 > 1$  due to  $Z \neq Z'$ . Then  $(X, Y) \in K(Z, Z')$  implies

$$(s_2 - 1) \|Q - (s_2 - t)(s_2 - 1)^{-1} Y\|_1 \leq (s_2 - 1) \|P - (s_2 - t)(s_2 - 1)^{-1} Z'\|_1 \tag{39}$$

for all reals  $t$  (since  $\|X - tY\|_1 = 1 + |t| = \|Z - tZ'\|_1$  for  $t < 0$ ), i.e. (39) implies

$$(Q, Y) \in K(P, Z'). \tag{40}$$

Again using 3, Lemma 3 we find from (40)

$$(Q, Y) \in K_0(P, Z'). \tag{41}$$

By (38) and arguments similar to (34)–(36),

$$(X, Y) \in K_0(Z, Z'). \tag{42}$$

Thirdly, let

$$s_2(Z, Z') = s_2(X, Y) = +\infty. \tag{43}$$

Then by 2 (8)  $Z'$  and  $Y$  are orthoprojections and 3, Lemma 3 becomes applicable.

This leads to (28) again.

At last, assume (27) holds with  $s_1(X, Y) = 1$ . Then due to 2 (9), (10) we see that  $X = Y$  and the application of 3, Lemma 1 leads to (28). This proves Lemma 2. q.e.d.

### Conclusion

By Lemma 2 and 3, Lemma 2 we are assured that

$$(X, Y) \in \text{ex}K(Z, Z') \quad \text{implies} \quad (X, Y) \in K_0(Z, Z'). \tag{44}$$

Then, since  $K_0(Z, Z')$  is closed and convex, we conclude that

$$K(Z, Z') = \overline{\text{conv ex}K(Z, Z')} \subset K_0(Z, Z'). \tag{45}$$

By our remark following the theorem in 1 the inclusion  $K_0(Z, Z') \subset K(Z, Z')$  is obviously valid, so by (45)  $K(Z, Z') = K_0(Z, Z')$  must to be true. This completes the proof of our theorem. q.e.d.

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