

QUANTUM MAGIC SQUARES: DILATIONS AND THEIR LIMITATIONS

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ABSTRACT. Quantum permutation matrices and quantum magic squares are generalizations of permutation matrices and magic squares, where the entries are no longer numbers but elements from arbitrary (non-commutative) algebras. The famous Birkhoff–von Neumann Theorem characterizes magic squares as convex combinations of permutation matrices. In the non-commutative case, the corresponding question is: Does every quantum magic square belong to the matrix convex hull of quantum permutation matrices? That is, does every quantum magic square dilate to a quantum permutation matrix? Here we show that this is false even in the simplest non-commutative case. We also classify the quantum magic squares that dilate to a quantum permutation matrix with commuting entries, and prove a quantitative lower bound on the diameter of this set. Finally, we conclude that not all Arveson extreme points of the free spectrahedron of quantum magic squares are quantum permutation matrices.

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1. INTRODUCTION

A magic square is a square of nonnegative numbers with the property that every row and column sums to the same value. (Often it is additionally required that the diagonals also sum to this value, but we will not require this here). If the number they sum to is one, magic squares are also called doubly stochastic matrices. Throughout this work we will use the words magic square and doubly stochastic matrix interchangeably, i.e. we always assume that all rows and columns of our matrices sum to one.

The Birkhoff–von Neumann Theorem is a central result in this context, which says that every magic square is a convex combination of permutation matrices—see for example [3]. Furthermore, the permutation matrices constitute precisely the vertices of the polytope of all magic squares. This result is a beautiful and useful characterization of magic squares, with applications in the theory of Markov chains, matrix approximations, the graph isomorphism problem, market design and many more—see for example [4, 5].

Several generalizations of magic squares and their corresponding Birkhoff–von Neumann Theorem have been proposed in the literature. One such generalization are unital quantum channels, that is, completely positive and trace preserving linear maps which map the identity to itself. It is easy to see that (the diagonal elements of) unital quantum channels that map diagonal matrices to diagonal matrices correspond to magic squares. A version of the Birkhoff–von Neumann Theorem for unital quantum channels has been shown to fail in [13], and an asymptotic version thereof has also been shown to fail in [11]; see also [15] for a detailed analysis.

In this work we consider a different generalization of magic squares, which is inspired by non-commutative semialgebraic geometry and free convexity (see e.g. [16]). Namely, we define magic squares over an algebra \mathcal{A} as matrices containing positive elements from \mathcal{A} , and such that every row and column sums to the identity element in \mathcal{A} . We call such matrices *quantum magic squares*. If, additionally, every element is a projector, then the magic square is called a *quantum permutation matrix* (also called magic unitary in [14, 18]). For readers familiar with quantum information theory, a magic square over the algebra of complex matrices of size $s \times s$, $\text{Mat}_s(\mathbb{C})$, contains a positive operator valued measurement (POVM) in each row and in each column, and a quantum permutation matrix contains a projective measurement in each row and column. If the algebra \mathcal{A} is simply the complex numbers \mathbb{C} , then quantum magic squares and quantum permutation matrices coincide with magic squares and permutation matrices, respectively. We refer to this special case as the “classical” case, intuitively because quantum behaviour is associated to non-commutativity, and thereby to non-commutative algebras such as $\text{Mat}_s(\mathbb{C})$. Note that quantum permutation matrices have been studied in several contexts: as $*$ -representations of the quantum permutation group [2], to characterize quantum isomorphism of graphs [1] and to represent perfect quantum strategies for non-local games [14, 18].

To be more specific, in this work we consider the free (i.e. non-commutative) semialgebraic sets of all magic squares and of all quantum permutation matrices over matrix algebras. The first level of these free semialgebraic sets corresponds to the classical case: we recover the sets of magic squares and of permutation matrices, respectively. We then investigate the *matrix convex hull* of the quantum permutation matrices. This is a special notion of convexity which is well-adapted to non-commutative sets, as it relates the different matrix levels by isometric conjugations. In a more operator theoretic formulation, we investigate which quantum magic squares admit a *dilation* to a quantum permutation matrix. While a single POVM can be dilated to a projective measurement via Stinespring's Dilation Theorem [17], this does not imply that a quantum magic square can be dilated to a quantum permutation matrix, since the former contains a POVM in every row and every column, and we are asking for a *simultaneous* dilation of all of them.

To address these questions, we first completely characterize the matrix convex hull of all quantum permutation matrices with *commuting* entries (see Section 2.2 for a definition of the matrix convex hull). Namely, we show that a quantum magic square dilates to a quantum permutation matrix with commuting entries if and only if it is *semiclassical* (Theorem 12). Semiclassical means that it can be expressed as a sum of tensor products of permutation matrices and positive semidefinite matrices. Throughout this paper, we denote the number of rows (which equals the number of columns) of the quantum magic square by n . When the algebra \mathcal{A} is $\text{Mat}_s(\mathbb{C})$ with $s \geq 2$, we show that there exist quantum magic squares of all sizes $n \geq 3$ which are not semiclassical (Corollary 15). We also prove a lower bound on the diameter of the free convex set of semiclassical magic squares (Theorem 12).

The matrix convex hull of *all* quantum permutation matrices is much harder to describe. We prove that for every size $n \geq 3$ there exist quantum magic squares of size n over $\text{Mat}_2(\mathbb{C})$ that do not dilate to any quantum permutation matrix (Theorem 19). This means that the matrix convex hull of the set of quantum permutation matrices is strictly contained in the set of all quantum magic squares. We conclude that all quantum permutation matrices are Arveson extreme points (see Definition 16) of the free spectrahedron of quantum magic squares, but that for $n \geq 3$ not every Arveson extreme point is a quantum permutation matrix.

This paper is organized as follows. Section 2 contains preliminary material needed in the course of the paper, including quantum magic squares and permutation matrices, basic concepts of non-commutative semialgebraic geometry and convexity, and operator systems. Section 3 contains our main results. In the first part (Section 3.1), we give a complete characterization of the quantum magic squares that dilate to a quantum permutation matrix with commuting entries (Theorem 12), we prove a lower bound on the diameter of the set of these quantum magic squares, and we conclude that there exist non-semiclassical quantum magic squares of any size $n \geq 3$, and non-semiclassical

quantum permutation matrices of any size $n \geq 4$ (Corollary 15). In the second part (Section 3.2), we show that for any $n \geq 3$ there exist quantum magic squares of size n that do not dilate to any quantum permutation matrix (Theorem 19), and we conclude that quantum permutation matrices are Arveson extreme points of the set of all quantum magic squares, but not every Arveson extreme point is of that form (Corollary 17).

2. PRELIMINARIES

In this section we define and characterize quantum magic squares and quantum permutation matrices (Section 2.1), free semialgebraic sets and matrix convex hulls (Section 2.2), and certain operator systems (Section 2.3).

2.1. Quantum magic squares and quantum permutation matrices.

Throughout this paper let \mathcal{A} be a C^* -algebra. The real vector space of Hermitian elements in \mathcal{A} is denoted by \mathcal{A}_{her} , and the closed convex cone of positive elements in \mathcal{A}_{her} by \mathcal{A}^+ . We will mostly assume that $\mathcal{A} = \text{Mat}_s(\mathbb{C})$, the C^* -algebra of complex matrices of size $s \times s$. Instead of $\text{Mat}_s(\mathbb{C})_{\text{her}}$ we write $\text{Her}_s(\mathbb{C})$, and instead of $a \in \text{Mat}_s(\mathbb{C})^+$ we just write $a \geq 0$.

Definition 1. Let $n \in \mathbb{N}$ and $A = (a_{ij})_{i,j} \in \text{Mat}_n(\mathcal{A})$.

(i) A is called a magic square over \mathcal{A} if all $a_{ij} \in \mathcal{A}^+$ and all rows and columns of A sum to 1, the identity element in \mathcal{A} . A magic square over some algebra \mathcal{A} is called a quantum magic square.

(ii) A magic square over \mathcal{A} is called a permutation matrix over \mathcal{A} if all a_{ij} are projectors, i.e. fulfill $a_{ij}^2 = a_{ij}$. A permutation matrix over some \mathcal{A} is called a quantum permutation matrix.

Remark 2. (i) Every quantum permutation matrix is a unitary in the sense that

$$A^*A = AA^* = I_n \in \text{Mat}_n(\mathcal{A}).$$

Although the defining conditions only require

$$\sum_j a_{ij} = \sum_i a_{ij} = 1$$

for all i, j , the fact that the a_{ij} are projectors in a C^* -algebra implies that

$$a_{ij}a_{ik} = 0 = a_{ji}a_{ki}$$

for all i and $j \neq k$.

(ii) In the case $\mathcal{A} = \mathbb{C}$, quantum magic squares become magic squares and quantum permutations become permutation matrices (that is, a matrix with exactly one 1 in every row and column, and 0 elsewhere). The well-known Birkhoff–von Neumann Theorem states that permutation matrices are precisely the vertices of the polytope of all magic squares, see for example [3, 19]. In particular, every magic square is a convex combination of permutation matrices. This holds for all matrix sizes $n \geq 1$.

(iii) For matrix size $n = 1$ and any \mathcal{A} , the only magic square over \mathcal{A} is (1). For $n = 2$ every magic square over \mathcal{A} is of the form

$$\begin{pmatrix} a & 1-a \\ 1-a & a \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes a + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes (1-a)$$

with $a, 1-a \in \mathcal{A}^+$. Whether this is a convex combination of permutation matrices over \mathcal{A} just depends on whether a is a convex combination of projectors in \mathcal{A} . In case that $\mathcal{A} = \text{Mat}_s(\mathbb{C})$ is a matrix algebra, this was first shown to hold in [6] for any such a . If $\mathcal{A} = \mathcal{B}(\mathcal{H})$ is the algebra of bounded operators on an infinite-dimensional Hilbert space \mathcal{H} , this is not true with *finite* convex combinations [9]. But from the spectral theorem it follows that it holds up to the closure, even over any C^* -algebra. So the Birkhoff–von Neumann Theorem holds for matrices of size 2 over matrix algebras with convex combinations, and over arbitrary C^* -algebras with convex combinations and closures. This is known to fail for $n \geq 3$ and we will prove a stronger statement below.

We denote the permutation group of n elements by S_n , as customary.

Definition 3. A magic square $A \in \text{Mat}_n(\mathcal{A})$ over \mathcal{A} is called semiclassical if it can be written as

$$A = \sum_{\pi \in S_n} P_\pi \otimes q_\pi,$$

where $P_\pi \in \text{Mat}_n(\mathbb{C})$ are permutation matrices and $q_\pi \in \mathcal{A}^+$ (with $\sum_\pi q_\pi = 1$).

Remark 4. (i) For $n = 1, 2$ all quantum magic squares are semiclassical. For $\mathcal{A} = \mathbb{C}$ and all n , all magic squares over \mathcal{A} are semiclassical. We will show in Corollary 15 that for $n \geq 3$ and $\mathcal{A} = \text{Mat}_s(\mathbb{C})$ with $s \geq 2$ there exist magic squares over \mathcal{A} that are not semiclassical. There even exist non-semiclassical quantum permutation matrices, at least for $n \geq 4$ and $s \geq 2$.

(ii) Let $A = (a_{ij}) \in \text{Mat}_n(\mathcal{A})$ be a magic square over \mathcal{A} and let $\rho: S_n \rightarrow \{1, \dots, n!\}$ be a bijection. We set

$$B := \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad C_{ij} := \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{ij} \\ 0 & 0 & 0 & E_{ij}^t & 0 \end{pmatrix},$$

$$D_\pi := \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_{\rho(\pi)\rho(\pi)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -P_\pi \\ 0 & 0 & 0 & -P_\pi^t & 0 \end{pmatrix}$$

where E_{kl} denotes the canonical basis of either $\text{Mat}_n(\mathbb{C})$ or $\text{Mat}_{n!}(\mathbb{C})$. Then A is semiclassical if and only if there exist $q_\pi \in \mathcal{A}$ for all $\pi \in S_n$ such that

$$B \otimes 1_{\mathcal{A}} + \sum_{i,j=1}^n C_{ij} \otimes a_{ij} + \sum_{\pi \in S_n} D_\pi \otimes q_\pi$$

is an element of $\text{Mat}_{n!+2n+2}(\mathcal{A})^+$. Thus, for $\mathcal{A} = \text{Mat}_s(\mathbb{C})$ checking whether a magic square is semiclassical reduces to a semidefinite program.

2.2. Matrix convex hulls. In this section we consider non-commutative sets, which are sets of matrix tuples, for any size of the matrices. As we will see, the set of quantum magic squares and of quantum permutation matrices are examples of such sets.

Definition 5. For $n, s \geq 1$ we define

$$\begin{aligned} \mathcal{M}_s^{(n)} &:= \{A \in \text{Mat}_n(\text{Her}_s(\mathbb{C})) \mid A \text{ quantum magic square}\} \\ \mathcal{P}_s^{(n)} &:= \{A \in \text{Mat}_n(\text{Her}_s(\mathbb{C})) \mid A \text{ quantum permutation matrix}\} \\ \mathcal{CP}_s^{(n)} &:= \left\{A \in \mathcal{P}_s^{(n)} \mid \text{all entries of } A \text{ commute}\right\} \end{aligned}$$

and

$$\mathcal{M}^{(n)} := \bigcup_{s \geq 1} \mathcal{M}_s^{(n)} \quad \mathcal{P}^{(n)} := \bigcup_{s \geq 1} \mathcal{P}_s^{(n)} \quad \mathcal{CP}^{(n)} := \bigcup_{s \geq 1} \mathcal{CP}_s^{(n)}.$$

We have the obvious inclusions

$$\mathcal{CP}^{(n)} \subseteq \mathcal{P}^{(n)} \subseteq \mathcal{M}^{(n)}.$$

For $n \leq 3$ we have

$$\mathcal{CP}^{(n)} = \mathcal{P}^{(n)}.$$

This is clear for $n = 1, 2$ and for $n = 3$ a nice elementary proof can be found in [14]. For $n \geq 4$

$$\mathcal{CP}^{(n)} \subsetneq \mathcal{P}^{(n)}$$

holds, which can easily be seen by taking a block diagonal sum of two quantum permutations of size 2 each.

As customary, we use $\text{Mat}_{s,t}(\mathbb{C})$ to denote the set of matrices of size $s \times t$ over the complex numbers.

Definition 6. For each $s \geq 1$ let some set $R_s \subseteq \text{Her}_s(\mathbb{C})^m$ be given. Then $R = \bigcup_{s \geq 1} R_s$ is called matrix convex if for all $r, s_i, t \geq 1$, $a^{(i)} \in R_{s_i}$ for $i = 1, \dots, r$ and $v_i \in \text{Mat}_{s_i, t}(\mathbb{C})$ with $\sum_{i=1}^r v_i^* v_i = I_t$,

$$\sum_{i=1}^r v_i^* a^{(i)} v_i \in R_t$$

holds. Here, compression of the m -tuple $a^{(i)}$ by v_i is meant entrywise. That is, we identify $\text{Her}_s(\mathbb{C})^m$ with $\text{Mat}_{1,m}(\mathbb{C}) \otimes \text{Her}_s(\mathbb{C})$ so that $v_i^* a^{(i)} v_i$ is identified with $(1 \otimes v_i^*) a^{(i)} (I_m \otimes v_i)$.

For more information on matrix convexity, see e.g. [7].

Remark 7. (i) If $R = \bigcup_{s \geq 1} R_s$ is matrix convex, then each R_s is convex in the standard sense. But the converse is generally not true, that is, being matrix convex is generally a stronger requirement than simply being convex at each level s .

(ii) The condition $\sum_{i=1}^r v_i^* a^{(i)} v_i$ can be written as $v^* a v$ by defining

$$v = (v_1, \dots, v_r)^t$$

and

$$a = \left(\bigoplus_{i=1}^r a_1^{(i)}, \dots, \bigoplus_{i=1}^r a_m^{(i)} \right),$$

where we have written $a^{(i)} = (a_1^{(i)}, \dots, a_m^{(i)})$. If the set R is closed under direct sums, then $a \in R$, and thus for these sets the definition of matrix convexity can be simplified to include this single summand. One example of a set closed under direct sums are free semialgebraic sets, i.e. sets defined by non-commutative polynomial inequalities (see for example [16] for more information).

(iii) Intersections of matrix convex sets are matrix convex. It follows that for every set $R = \bigcup_{s \geq 1} R_s$ there exists the matrix convex hull, i.e. the smallest matrix convex superset, which is obtained by adding all compressions of elements from R as in Definition 6, and which we denote by $\text{mconv}(R)$.

Example 8. The set $\mathcal{M}^{(n)}$ of quantum magic squares is matrix convex. For $n \geq 2$ the sets $\mathcal{CP}^{(n)}$ and $\mathcal{P}^{(n)}$ are not. We obtain

$$\text{mconv}(\mathcal{CP}^{(n)}) \subseteq \text{mconv}(\mathcal{P}^{(n)}) \subseteq \mathcal{M}^{(n)}.$$

For $n \leq 2$ these inclusions are all equalities. For $n = 2$ this follows from Remark 2 (iii) and Remark 7 (i). For $n = 3$ the inclusion on the left is an equality.

2.3. Magic cones and operator systems. Let $\mathcal{V}^{(n)} \subseteq \text{Mat}_n(\mathbb{C})$ be the space of all matrices with constant row and column sums, equipped with the involution of entrywise conjugation. Let

$$\mathcal{C}^{(n)} \subseteq \mathcal{V}_{\text{her}}^{(n)}$$

be the convex cone of real and entrywise nonnegative matrices from $\mathcal{V}^{(n)}$, that is, the set of magic squares in the non-normalized sense. We call $\mathcal{C}^{(n)}$ the *magic cone*.

Lemma 9. (i) $\mathcal{V}^{(n)}$ is spanned over \mathbb{C} by the permutation matrices, $\mathcal{V}_{\text{her}}^{(n)}$ is spanned over \mathbb{R} by the permutation matrices, and

$$\dim_{\mathbb{C}}(\mathcal{V}^{(n)}) = \dim_{\mathbb{R}}(\mathcal{V}_{\text{her}}^{(n)}) = (n-1)^2 + 1.$$

(ii) $\mathcal{C}^{(n)}$ is a polyhedral cone that does not contain a full line in $\mathcal{V}_{\text{her}}^{(n)}$, and the all-ones matrix is an interior point.

(iii) The extreme rays of $\mathcal{C}^{(n)}$ are precisely the rays spanned by the permutation matrices, of which there are $n!$ many. For $n \geq 3$, $\mathcal{C}^{(n)}$ has precisely n^2 facets, defined by the inequalities $x_{ij} \geq 0$ on the matrix entries, and $\mathcal{C}^{(n)}$ is not a simplex cone (i.e. the number of extreme rays exceeds its dimension).

Proof. All statements are easy observations or straightforward translations of the corresponding well-known facts about the Birkhoff polytope, see for example [3, 19]. \square

We now introduce the smallest and the largest operator system over the magic cone $\mathcal{C}^{(n)}$, and collect some of their properties. We refer the reader to [10] for more detailed explanations of these notions.

Definition 10. (i) For $s \in \mathbb{N}$ we define

$$\mathcal{S}_s^{(n)} := \left\{ \sum_{\pi \in S_n} P_\pi \otimes q_\pi \mid q_\pi \in \text{Mat}_s(\mathbb{C})^+ \right\}$$

where $P_\pi \in \text{Mat}_n(\mathbb{C})$ are the permutation matrices, and understand this convex cone as a subset of the Hermitian part of

$$\mathcal{V}^{(n)} \otimes \text{Mat}_s(\mathbb{C}) \subseteq \text{Mat}_n(\text{Mat}_s(\mathbb{C})).$$

We call

$$\mathcal{S}^{(n)} := \bigcup_{s \geq 1} \mathcal{S}_s^{(n)}$$

the smallest magic operator system.

(ii) For $s \in \mathbb{N}$ we define

$$\mathcal{L}_s^{(n)} := \left\{ A \in (\mathcal{V}^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}} \mid \forall v \in \mathbb{C}^s : (I_n \otimes v)^* A (I_n \otimes v) \in \mathcal{C}^{(n)} \right\}$$

and call

$$\mathcal{L}^{(n)} := \bigcup_{s \geq 1} \mathcal{L}_s^{(n)}$$

the largest magic operator system.

Remark 11. (i) $\mathcal{S}^{(n)}$ and $\mathcal{L}^{(n)}$ are really the smallest/largest abstract operator systems over $\mathcal{C}^{(n)}$, as defined in [10]. The only difference is that we consider $\mathcal{V}^{(n)} \otimes \text{Mat}_s(\mathbb{C})$ as a subspace of $\text{Mat}_n(\text{Mat}_s(\mathbb{C}))$, instead of identifying it with $\text{Mat}_s(\mathcal{V}^{(n)})$.

(ii) Magic squares of size n over $\text{Mat}_s(\mathbb{C})$ are precisely the elements from $\mathcal{L}_s^{(n)}$ with the additional property that every row and column sums to $I_s \in \text{Mat}_s(\mathbb{C})$. Such a quantum magic square is semiclassical if and only if it belongs to $\mathcal{S}_s^{(n)}$.

(iii) From Lemma 9 and [12, Theorem 1] it follows that for $n \leq 2$ we have $\mathcal{S}^{(n)} = \mathcal{L}^{(n)}$, but

$$\mathcal{S}_s^{(n)} \subsetneq \mathcal{L}_s^{(n)}$$

for all $n \geq 3$ and $s \geq 2$.

3. DILATIONS OF QUANTUM MAGIC SQUARES

In this section we present the main results of this paper. Namely, we characterize semiclassical quantum magic squares (Section 3.1), and the matrix convex hull of quantum permutations (Section 3.2).

3.1. Characterization of semiclassical quantum magic squares. The following is our main result concerning the characterization of semiclassical quantum magic squares.

Theorem 12. *Let $a = (a_{ij}) \in \mathcal{M}_s^{(n)}$ be a quantum magic square.*

(i) *Let \mathbb{C}^{S_n} be the C^* -algebra of all functions $S_n \rightarrow \mathbb{C}$ and let $f_{ij} \in \mathbb{C}^{S_n}$ be defined as*

$$f_{ij}(\pi) := \begin{cases} 1 & : \pi(i) = j \\ 0 & : \text{else} \end{cases}$$

Then the following are equivalent:

(a) *a is semiclassical*

(b) *$a \in \text{mconv}(\mathcal{CP}^{(n)})$*

(c) *There is a positive unital $*$ -linear map $\phi: \mathbb{C}^{S_n} \rightarrow \text{Mat}_s(\mathbb{C})$ with $\phi(f_{ij}) = a_{ij}$.*

(ii) *If*

$$\sum_{k=1}^n a_{k,\pi(k)} \geq \frac{n-2}{n-1} \cdot I_s$$

for all $\pi \in S_n$, then a is semiclassical.

Proof. (i): For “(a) \Rightarrow (b)” write

$$a = \sum_{\pi} P_{\pi} \otimes q_{\pi}$$

with permutation matrices $P_{\pi} = (p_{ij}^{\pi})_{i,j}$ and $q_{\pi} = v_{\pi}^* v_{\pi}$ for certain $v_{\pi} \in \text{Mat}_s(\mathbb{C})$. Set

$$\begin{aligned} u_{ij} &:= \text{diag}(p_{ij}^{\pi} I_s \mid \pi \in S_n) \in \text{Mat}_{n!s}(\mathbb{C}) \\ u &:= (u_{ij})_{i,j} \in \text{Mat}_n(\text{Mat}_{n!s}(\mathbb{C})) \\ v &:= (v_{\pi})_{\pi \in S_n} \in \text{Mat}_{n!s,s}(\mathbb{C}). \end{aligned}$$

Then v is easily checked to be an isometry (using that rows and columns of a sum to I_s), u to be a quantum permutation matrix with commuting entries, and $v^* u_{ij} v = a_{ij}$ for all i, j .

For “(b) \Rightarrow (c)” let $(u_{ij}) \in \mathcal{CP}_t^{(n)}$ and $v \in \text{Mat}_{t,s}(\mathbb{C})$ such that $v^* v = I_s$ and

$$a_{ij} = v^* u_{ij} v.$$

Now we define the map

$$\psi: \mathbb{C}^{S_n} \rightarrow \text{Mat}_t(\mathbb{C}), \quad f \mapsto \sum_{\pi \in S_n} f(\pi) \cdot \prod_{k=1}^n u_{k,\pi(k)}.$$

We want to show that ψ is a unital $*$ -algebra-homomorphism with $\psi(f_{ij}) = u_{ij}$. The $*$ -linearity is easy to see. Since the u_{ij} commute we have

$$\psi(f)\psi(g) = \sum_{\pi, \sigma \in S_n} f(\pi)g(\sigma) \cdot \prod_{k=1}^n u_{k,\pi(k)}u_{k,\sigma(k)}.$$

Now if $\pi \neq \sigma$, then there is an index k with $\pi(k) \neq \sigma(k)$. Since (u_{ij}) is a quantum permutation matrix, we get from Remark 2 (i) that $u_{k,\pi(k)}u_{k,\sigma(k)} = 0$. Thus

$$\psi(f)\psi(g) = \sum_{\pi \in S_n} f(\pi)g(\pi) \cdot \prod_{k=1}^n u_{k,\pi(k)}^2 = \sum_{\pi \in S_n} (f \cdot g)(\pi) \cdot \prod_{k=1}^n u_{k,\pi(k)} = \psi(f \cdot g).$$

In order to compute $\psi(f_{ij})$ we first note that the sum in the definition of ψ does not change when we extend it to non-injective maps. This follows from a similar argument as above. Now for $[n] := \{1, \dots, n\}$ we have

$$\begin{aligned} \psi(f_{nn}) &= \sum_{\pi \in S_n} f_{nn}(\pi) \cdot \prod_{k=1}^n u_{k,\pi(k)} = \sum_{\pi: [n] \rightarrow [n], \pi(n)=n} \prod_{k=1}^n u_{k,\pi(k)} \\ &= u_{nn} \sum_{\pi: [n-1] \rightarrow [n]} \prod_{k=1}^{n-1} u_{k,\pi(k)} = u_{nn} \cdot \sum_{\tau_1=1}^n \cdots \sum_{\tau_{n-1}=1}^n \prod_{k=1}^{n-1} u_{k,\tau_k} \\ &= u_{nn} \cdot \prod_{k=1}^{n-1} \sum_{\tau=1}^n u_{k,\tau} = u_{nn} \end{aligned}$$

The last equality follows from the fact that the columns of (u_{ij}) sum to I_t . Similarly we can compute $\psi(f_{ij}) = u_{ij}$ for all i, j . Finally, ψ is unital because both (f_{ij}) and (u_{ij}) are quantum permutation matrices. Now the map $\phi(f) := v^* \psi(f) v$ satisfies the requirements of (c).

For “(c) \Rightarrow (a)” let $\delta_\pi \in \mathbb{C}^{S_n}$ be the characteristic function of π , i.e. the function that takes the value 1 on π and 0 on all other permutations. From $\delta_\pi \geq 0$ and the properties of ϕ we obtain $q_\pi := \phi(\delta_\pi) \geq 0$ and $\sum_\pi q_\pi = I_s$. Now we compute

$$\begin{aligned} a &= \sum_{i,j=1}^n E_{ij} \otimes a_{ij} = (\text{id} \otimes \phi) \left(\sum_{i,j=1}^n E_{ij} \otimes f_{ij} \right) \\ &= (\text{id} \otimes \phi) \left(\sum_{\pi \in S_n} P_\pi \otimes \delta_\pi \right) = \sum_{\pi \in S_n} P_\pi \otimes q_\pi. \end{aligned}$$

Hence, a is semiclassical.

(ii): Under the given assumption a straightforward computation shows that

$$\phi: \mathbb{C}^{S_n} \rightarrow \text{Mat}_s(\mathbb{C}), \quad \delta_\pi \mapsto \frac{1}{(n-2)!n} \left(\left(\sum_{k=1}^n a_{k,\pi(k)} \right) - \frac{n-2}{n-1} \cdot I_s \right)$$

is a positive unital $*$ -linear map with $\phi(f_{ij}) = a_{ij}$. Thus, the claim follows from (i). \square

Remark 13. (i) Note that the condition in Theorem 12 (ii) is fulfilled by the constant quantum magic square $(\frac{1}{n}I_s)_{i,j}$, which is a relative interior point of $\mathcal{M}_s^{(n)}$. So Theorem 12 (ii) can be understood as a lower bound on the diameter of the set of semiclassical quantum magic squares inside $\mathcal{M}^{(n)}$.

(ii) Also note that Theorem 12 (i) together with Remark 4 (ii) yields an efficient way for checking membership in $\text{mconv}(\mathcal{CP}^{(n)})$.

Finally, in order to obtain the desired corollary, we need the following preparatory lemma.

Lemma 14. *Let $u \in \text{Mat}_s(\mathbb{C})$ be a projector, $0 \leq w \leq I_t \in \text{Mat}_t(\mathbb{C})$ (i.e. w is a positive semidefinite contraction) and $v \in \text{Mat}_{t,s}(\mathbb{C})$ an isometry with*

$$u = v^* w v.$$

Then w is the direct sum of u and some contraction $0 \leq p \leq I_{t-s}$ with respect to the decomposition $\mathbb{C}^t = v\mathbb{C}^s \oplus (v\mathbb{C}^s)^\perp$.

Proof. With respect to the given decomposition we write

$$w = \begin{pmatrix} u & r \\ r^* & p \end{pmatrix}$$

and compute

$$\begin{aligned} \begin{pmatrix} u & r \\ r^* & p \end{pmatrix} = w \geq w^2 &= \begin{pmatrix} u^2 + rr^* & ur + rp \\ r^*u + pr^* & r^*r + p^2 \end{pmatrix} \\ &= \begin{pmatrix} u + rr^* & ur + rp \\ r^*u + pr^* & r^*r + p^2 \end{pmatrix}. \end{aligned}$$

We obtain $r = 0$ and $p \geq p^2$. \square

Corollary 15. (i) *For every $n \geq 3$ and $s \geq 2$ there exist quantum magic squares in $\mathcal{M}_s^{(n)}$ which are not semiclassical. In particular*

$$\text{mconv}(\mathcal{CP}^{(n)}) \subsetneq \mathcal{M}^{(n)}.$$

(ii) *Every quantum permutation matrix of size $n \leq 3$ is semiclassical, but for every $n \geq 4, s \geq 2$ there exist quantum permutation matrices which are not semiclassical.*

Proof. (i) From Remark 11 (iii) we know that

$$\mathcal{S}_s^{(n)} \subsetneq \mathcal{L}_s^{(n)}$$

is a strict inclusion of closed convex cones with non-empty interior. So there must be an element $A \in \mathcal{L}_s^{(n)} \setminus \mathcal{S}_s^{(n)}$ for which the row and column sum is a positive definite matrix $0 < a \in \text{Mat}_s(\mathbb{C})^+$. Thus, there exists an invertible matrix $w \in \text{Mat}_s(\mathbb{C})$ such that $w^*aw = I_s$. Replacing the entries a_{ij} of A by $w^*a_{ij}w$ leads to a quantum magic square that is clearly not contained in $\mathcal{S}_s^{(n)}$, meaning that it is not semiclassical.

(ii) For $n \leq 3$ we have $\mathcal{CP}^{(n)} = \mathcal{P}^{(n)}$, from which the first statement follows. For $n \geq 4$ and $s \geq 2$ there exist quantum permutation matrices $U = (u_{ij})_{i,j} \in \mathcal{P}_s^{(n)} \setminus \mathcal{CP}_s^{(n)}$. One can take for example a block-diagonal sum of two suitable smaller quantum permutation matrices. If such U was semiclassical, it would admit a dilation as in Theorem 12 (i), i.e. $u_{ij} = v^*w_{ij}v$ with $(w_{ij})_{i,j} \in \mathcal{CP}^{(n)}$. By Lemma 14 we can assume

$$w_{ij} = \begin{pmatrix} u_{ij} & 0 \\ 0 & p_{ij} \end{pmatrix}$$

which contradicts the fact that the u_{ij} do not all commute. \square

We conclude this section with some first insights on the boundary structure of $\mathcal{M}^{(n)}$.

Definition 16. Let $R = \bigcup_{s \geq 1} R_s$ be a matrix convex set (as in Definition 6). Then $A = (a_{ij})_{i,j} \in R_s$ is an Arveson extreme point of R if whenever A dilates to $B = (b_{ij})_{i,j} \in R_t$, then each a_{ij} is a direct summand of b_{ij} up to a simultaneous unitary conjugation.

In words, this means that A only admits “trivial” dilations, that is, of the form

$$b_{ij} = \begin{pmatrix} a_{ij} & 0 \\ 0 & c_{ij} \end{pmatrix},$$

see also [8] for more details.

Corollary 17. (i) Every quantum permutation matrix in $\mathcal{P}^{(n)}$ is an Arveson extreme point of the matrix convex set $\mathcal{M}^{(n)}$ of all quantum magic squares.

(ii) $\mathcal{M}^{(n)}$ is the matrix convex hull of its Arveson extreme points.

Proof. (i) Let $U = (u_{ij})_{i,j} \in \mathcal{P}^{(n)}$ and assume $U = (v^*a_{ij}v)_{i,j}$ for some quantum magic square $A = (a_{ij})_{i,j} \in \mathcal{M}^{(n)}$ and an isometry v . Since A is a quantum magic square we have $0 \leq a_{ij} \leq I$ for all i, j . By Lemma 14, each a_{ij} splits off u_{ij} as a direct summand, and thus U is an Arveson extreme point.

(ii) Note that $\mathcal{M}^{(n)}$ is a compact free spectrahedron, i.e. definable by a linear matrix inequality (even by finitely many linear inequalities with scalar coefficients). In [8] it is shown that the matrix convex hull of the absolute

extreme points, and in particular of the Arveson extreme points, is the full spectrahedron. \square

Remark 18. From Corollary 15 and Corollary 17 (ii) we can already conclude that *not* every Arveson extreme point of $\mathcal{M}^{(3)}$ is a quantum permutation matrix. In Corollary 22 we will generalize this result to $\mathcal{M}^{(n)}$ for arbitrary $n \geq 3$.

3.2. The matrix convex hull of quantum permutation matrices. Our main goal in this section is to prove the following result.

Theorem 19. *For every $n \geq 3$ we have $\text{mconv}(\mathcal{P}^{(n)}) \subsetneq \mathcal{M}^{(n)}$. The difference already appears at level $s = 2$.*

Note that for $n = 3$ the result follows from Corollary 15 (i) and the fact that $\mathcal{CP}^{(3)} = \mathcal{P}^{(3)}$. Proving the result for general $n \geq 4$ requires some more work, since we were not able to deduce it from an obvious embedding argument. We will instead establish a necessary condition for being in the matrix convex hull of $\mathcal{P}^{(n)}$ (Proposition 21), show its failure for a quantum magic square from $\mathcal{M}_2^{(3)}$, and see that this implies failure for obvious embeddings into quantum magic squares of larger size n .

Construction 20. Let $A = (a_{ij}) \in \mathcal{M}_s^{(n)}$. We define matrices $\text{col}(A)$ and $\text{diag}(A)$ by writing the entries of A in one column and on the diagonal of a matrix respectively, where pairs of indices are ordered lexicographically, i.e. in the order $(1, 1), (1, 2), (1, 3), \dots, (2, 1), (2, 2), \dots, (n, n)$. We can consider these matrices as elements of threefold tensor products as follows:

$$\begin{aligned} \text{col}(A) &:= \sum_{i,j=1}^n e_i \otimes e_j \otimes a_{ij} \in \mathbb{C}^n \otimes \mathbb{C}^n \otimes \text{Her}_s(\mathbb{C}) \\ \text{diag}(A) &:= \sum_{i,j=1}^n E_{ii} \otimes E_{jj} \otimes a_{ij} \in \text{Mat}_n(\mathbb{C}) \otimes \text{Mat}_n(\mathbb{C}) \otimes \text{Her}_s(\mathbb{C}) \end{aligned}$$

where e_i and E_{ij} denote the canonical basis of \mathbb{C}^n and $\text{Mat}_n(\mathbb{C})$, respectively. Now let

$$\varphi(A) := \text{diag}(A) - \text{col}(A) \text{col}(A)^* \in (\text{Mat}_n(\mathbb{C}) \otimes \text{Mat}_n(\mathbb{C}) \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}.$$

For example for $n = 2$ the matrix $\varphi(A)$ looks as follows:

$$\begin{pmatrix} a_{11} - a_{11}^2 & -a_{11}a_{12} & -a_{11}a_{21} & -a_{11}a_{22} \\ -a_{12}a_{11} & a_{12} - a_{12}^2 & -a_{12}a_{21} & -a_{12}a_{22} \\ -a_{21}a_{11} & -a_{21}a_{12} & a_{21} - a_{21}^2 & -a_{21}a_{22} \\ -a_{22}a_{11} & -a_{22}a_{12} & -a_{22}a_{21} & a_{22} - a_{22}^2 \end{pmatrix}$$

For $n \geq 3$ we further define the matrix

$$\psi(A) := \sum_{\substack{i,j,k,l=1 \\ i \neq j, k \neq l}}^n E_{ij} \otimes E_{kl} \otimes (-\alpha_n I_s + \beta_n a_{ik} + \beta_n a_{jl} + \gamma_n a_{il} + \gamma_n a_{jk})$$

where

$$\alpha_n := \frac{1}{(n-1)(n-2)}, \quad \beta_n := \frac{n-1}{n(n-2)}, \quad \gamma_n := \frac{1}{n(n-2)}.$$

△

We let $\mathcal{Z}^{(n)}$ denote the vector space of all matrices in $\text{Mat}_n(\mathbb{C})$ with zeros on the diagonal. Moreover, for $e := (1, \dots, 1)^t \in \mathbb{C}^n$ we define the following subspace of $\mathcal{Z}^{(n)}$:

$$\mathcal{Z}_e^{(n)} := \{z \in \mathcal{Z}^{(n)} \mid ze = z^*e = 0\}.$$

Proposition 21. (i) For all $A \in \mathcal{M}_s^{(n)}$ the following are equivalent:

$$\exists X \in (\mathcal{Z}^{(n)} \otimes \mathcal{Z}^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}: \quad \varphi(A) + X \geq 0 \quad (1)$$

$$\exists X \in (\mathcal{Z}_e^{(n)} \otimes \mathcal{Z}_e^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}: \quad \varphi(A) + \psi(A) + X \geq 0 \quad (2)$$

(ii) For $A \in \text{mconv}(\mathcal{P}^{(n)})_s$ the formulas (1) and (2) are true.

Proof. (i) By definition we have $\psi(A) \in (\mathcal{Z}^{(n)} \otimes \mathcal{Z}^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}$. Thus, the implication (2)⇒(1) is obvious. For the same reason, (1) implies the formula

$$\exists X \in (\mathcal{Z}^{(n)} \otimes \mathcal{Z}^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}: \quad \varphi(A) + \psi(A) + X \geq 0.$$

Hence, for the reverse implication it suffices to show that if X satisfies this formula, then $X \in (\mathcal{Z}_e^{(n)} \otimes \mathcal{Z}_e^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}$. Using the fact that $A \in \mathcal{M}_s^{(n)}$ one can easily verify that

$$0 = (\varphi(A) + \psi(A))(e \otimes e_i \otimes I_s)$$

for $i = 1, \dots, n$ ($\psi(A)$ is precisely designed for this to be true). Moreover, from $X \in (\mathcal{Z}^{(n)} \otimes \mathcal{Z}^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}$ it follows that

$$0 = (e \otimes e_i \otimes I_s)^* X (e \otimes e_i \otimes I_s).$$

Together we obtain

$$0 = (e \otimes e_i \otimes I_s)^* (\varphi(A) + \psi(A) + X) (e \otimes e_i \otimes I_s).$$

From this and $\varphi(A) + \psi(A) + X \geq 0$ we conclude, for example with the Cauchy–Schwarz inequality, that

$$0 = (\varphi(A) + \psi(A) + X)(e \otimes e_i \otimes I_s) = X(e \otimes e_i \otimes I_s).$$

Since X is Hermitian, the same is true if we multiply from the other side, and by symmetry it is also true if we swap e and e_i . Therefore we obtain $X \in (\mathcal{Z}_e^{(n)} \otimes \mathcal{Z}_e^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}$.

(ii) Let $A \in \text{mconv}(\mathcal{P}^{(n)})_s$. By Remark 7 (ii) there is a quantum permutation matrix $U = (u_{ij}) \in \mathcal{P}_t^{(n)}$ and an isometry $v \in \text{Mat}_{t,s}(\mathbb{C})$ such that

$$a_{ij} = v^* u_{ij} v$$

for all i, j . By conjugating the u_{ij} with a suitable unitary matrix if necessary, we may assume v to be of the form

$$v = \begin{pmatrix} I_s \\ 0 \end{pmatrix}.$$

Then the u_{ij} have the form

$$u_{ij} = \begin{pmatrix} a_{ij} & b_{ij}^* \\ b_{ij} & c_{ij} \end{pmatrix}$$

for some matrices $b_{ij} \in \text{Mat}_{t-s,s}(\mathbb{C})$ and $c_{ij} \in \text{Her}_{t-s}(\mathbb{C})$. Since the u_{ij} are projectors, we have $u_{ij}^2 = u_{ij}$ and from Remark 2 (i) we additionally know $u_{ij}u_{ik} = 0 = u_{ji}u_{ki}$ for $j \neq k$. This implies

$$\begin{aligned} b_{ij}^* b_{ij} &= a_{ij} - a_{ij}^2 \\ b_{ik}^* b_{ij} &= -a_{ik} a_{ij} \\ b_{ji}^* b_{ki} &= -a_{ji} a_{ki}. \end{aligned} \tag{3}$$

From the matrices b_{ij}^* , we construct a matrix B in the same way we constructed $\text{col}(A)$ from the a_{ij} , i.e. B is just the column containing the b_{ij}^* . Now let

$$X := BB^* - \varphi(A).$$

Then we have

$$\varphi(A) + X = BB^* \geq 0$$

and $X \in (\mathcal{Z}^{(n)} \otimes \mathcal{Z}^{(n)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}$ follows from (3). \square

Proof of Theorem 19. We show by induction on n that (1) cannot hold for all elements of $\mathcal{M}_2^{(n)}$. For $n = 3$ let

$$\begin{aligned} a_{11} &:= \frac{1}{3}I_2 + \frac{9}{62} \begin{pmatrix} -\frac{34}{93} & \frac{4}{5} + \frac{2i}{13} \\ \frac{4}{5} - \frac{2i}{13} & \frac{7}{16} \end{pmatrix} \\ a_{12} &:= \frac{1}{3}I_2 + \frac{9}{62} \begin{pmatrix} \frac{5}{6} & \frac{1}{3} - \frac{20i}{81} \\ \frac{1}{3} + \frac{20i}{81} & -\frac{41}{55} \end{pmatrix} \\ a_{21} &:= \frac{1}{3}I_2 + \frac{9}{62} \begin{pmatrix} -\frac{2}{3} & -\frac{25}{92} - \frac{3i}{7} \\ -\frac{25}{92} + \frac{3i}{7} & \frac{1}{34} \end{pmatrix} \\ a_{22} &:= \frac{1}{3}I_2 + \frac{9}{62} \begin{pmatrix} \frac{29}{30} & \frac{6}{35} - i \\ \frac{6}{35} + i & -\frac{5}{8} \end{pmatrix} \end{aligned}$$

and define $a_{13}, a_{23}, a_{31}, a_{32}, a_{33}$ such that $A = (a_{ij})$ is an element of $\mathcal{M}_2^{(3)}$. By Proposition 21 (i) it is enough to show that this specific A does not satisfy (2). Note that the space $\mathcal{Z}_e^{(3)}$ is one-dimensional with Hermitian generator

$$g := \begin{pmatrix} 0 & i & -i \\ -i & 0 & i \\ i & -i & 0 \end{pmatrix}.$$

Thus, it remains to be shown that the formula

$$\exists x \in \text{Her}_2(\mathbb{C}): \quad \varphi(A) + \psi(A) + g \otimes g \otimes x \geq 0$$

is false. Now let

$$\begin{aligned} B_0 &:= \varphi(A) + \psi(A), & B_1 &:= g \otimes g \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & B_2 &:= g \otimes g \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ B_3 &:= g \otimes g \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, & B_4 &:= g \otimes g \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

Then it suffices to find a matrix $Y \in (\text{Mat}_3(\mathbb{C}) \otimes \text{Mat}_3(\mathbb{C}) \otimes \text{Mat}_2(\mathbb{C}))_{\text{her}}$ such that

$$\begin{aligned} Y &\geq 0 \\ \text{tr}(YB_0) &< 0 \\ \text{tr}(YB_j) &= 0 \quad j = 1, 2, 3, 4. \end{aligned}$$

Such a matrix exists, which can be verified by the attached Mathematica™ file *Counterexample.nb*. Note that all computations are over $\mathbb{Q}[i]$ and thus exact.

Now let $n > 3$. By the induction hypothesis there is an element $A \in \mathcal{M}_2^{(n-1)}$ that does not satisfy (1). We claim that the same is true for

$$A' = \begin{pmatrix} A & 0 \\ 0 & I_2 \end{pmatrix} \in \mathcal{M}_2^{(n)}.$$

Let

$$v = \begin{pmatrix} I_{n-1} \\ 0 \end{pmatrix} \in \text{Mat}_{n,n-1}(\mathbb{C})$$

and let $X' \in (\mathcal{Z}^{(n)} \otimes \mathcal{Z}^{(n)} \otimes \text{Mat}_2(\mathbb{C}))_{\text{her}}$ be an arbitrary element. Then we have

$$X := (v \otimes v \otimes I_2)^* X' (v \otimes v \otimes I_2) \in (\mathcal{Z}^{(n-1)} \otimes \mathcal{Z}^{(n-1)} \otimes \text{Mat}_2(\mathbb{C}))_{\text{her}}$$

and

$$(v \otimes v \otimes I_2)^* (\varphi(A') + X') (v \otimes v \otimes I_2) = \varphi(A) + X \not\geq 0.$$

It follows that

$$\varphi(A') + X' \not\geq 0.$$

Since X' was arbitrary, the claim follows. \square

In Appendix A we provide an alternative proof of Theorem 19 which does not use this explicit example, but gives no information on the level at which the difference appears.

With Theorem 19 we can now generalize the result in Remark 18 about the boundary structure of $\mathcal{M}^{(3)}$ to $\mathcal{M}^{(n)}$ for arbitrary $n \geq 3$.

Corollary 22. *For $n \geq 3$ not every Arveson extreme point of $\mathcal{M}^{(n)}$ is a quantum permutation matrix.*

Proof. Follows from Corollary 17 (ii) and Theorem 19. \square

APPENDIX A. ALTERNATIVE PROOF OF THEOREM 19

In the proof of Theorem 19 we gave an explicit element $A \in \mathcal{M}_s^{(3)}$ that does not satisfy the constraint (1) from Proposition 21. In this appendix we give a conceptual proof that such an element A exists. However, in contrast to the original proof this does not show that we can choose $s = 2$. Recall from Construction 20 the definition of $\varphi(A)$ and $\psi(A)$.

Proposition 23. *There exists a natural number s and an element $A \in \mathcal{M}_s^{(3)}$ such that*

$$\forall X \in (\mathcal{Z}^{(3)} \otimes \mathcal{Z}^{(3)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}: \quad \varphi(A) + X \not\geq 0.$$

Proof. By Remark 18 there is an Arveson extreme point $A \in \mathcal{M}_s^{(3)}$ of $\mathcal{M}^{(3)}$ that is not a quantum permutation matrix. Without loss of generality we may assume that

$$a_{11} - a_{11}^2 \neq 0.$$

We show by contradiction that A satisfies the claim. So assume that there exists an $X \in (\mathcal{Z}^{(3)} \otimes \mathcal{Z}^{(3)} \otimes \text{Mat}_s(\mathbb{C}))_{\text{her}}$ such that

$$\varphi(A) + X \geq 0.$$

Then we can find a matrix B such that

$$\varphi(A) + X = BB^*.$$

We write B as

$$B = \sum_{i,j=1}^3 e_i \otimes e_j \otimes b_{ij}^*$$

with matrices $b_{ij} \in \text{Mat}_{t,s}(\mathbb{C})$ for some natural number t (cf. proof of Proposition 21). It follows that

$$b_{11}^* b_{11} = a_{11} - a_{11}^2 \neq 0.$$

In particular, we can find a vector $v \in \mathbb{C}^s$ such that

$$v^* b_{11}^* b_{11} v = 1.$$

On the other hand we obtain from $A \in \mathcal{M}^{(3)}$ that

$$\begin{aligned} (b_{i1} + b_{i2} + b_{i3})^* (b_{i1} + b_{i2} + b_{i3}) &= \sum_{k,l=1}^3 b_{ik}^* b_{il} = \sum_{k,l=1}^3 (\delta_{kl} a_{ik} - a_{ik} a_{il}) \\ &= \sum_{k=1}^3 (a_{ik} - a_{ik} \cdot I_s) = 0. \end{aligned}$$

This implies

$$b_{i1} + b_{i2} + b_{i3} = b_{1j} + b_{2j} + b_{3j} = 0 \tag{A1}$$

for all $i, j = 1, 2, 3$. For $i, j = 1, 2, 3$ let p_{ij} be the Moore–Penrose inverse of $a_{ij}^{\frac{1}{2}}$. Since the $a_{ij}^{\frac{1}{2}}$ are Hermitian, it is well known that p_{ij} is Hermitian as well and that

$$p_{ij}a_{ij}^{\frac{1}{2}} = a_{ij}^{\frac{1}{2}}p_{ij} \quad (\text{A2})$$

is the orthogonal projection onto $\ker(a_{ij})^{\perp}$. Since $b_{ij}^*b_{ij} = a_{ij} - a_{ij}^2$, this gives

$$b_{ij}p_{ij}a_{ij}^{\frac{1}{2}} = b_{ij}. \quad (\text{A3})$$

Our goal is now to show that there are real numbers $c_{ij} \geq 0$ such that the matrix $A' = (a'_{ij})$ with

$$a'_{ij} := \begin{pmatrix} a_{ij} & b_{ij}^*b_{11}v \\ v^*b_{11}^*b_{ij} & v^*b_{11}^*b_{ij}p_{ij}^2b_{ij}^*b_{11}v + c_{ij} \end{pmatrix} \in \text{Her}_{s+1}(\mathbb{C})$$

is an element of $\mathcal{M}_{s+1}^{(3)}$. If that is the case, then A cannot be an Arveson extreme point of $\mathcal{M}^{(3)}$ since $b_{11}^*b_{11}v \neq 0$ by our construction. So we arrive at a contradiction. Thus, it remains to be shown that $A' \in \mathcal{M}_{s+1}^{(3)}$, i.e. that $a'_{ij} \geq 0$ and that the sum of the a'_{ij} in each row and each column is I_{s+1} . For $a'_{ij} \geq 0$ we compute

$$\begin{aligned} 0 &\leq \begin{pmatrix} I_s & \\ v^*b_{11}^*b_{ij}p_{ij}^2 & \end{pmatrix} a_{ij} \begin{pmatrix} I_s & p_{ij}^2b_{ij}^*b_{11}v \\ & \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & c_{ij} \end{pmatrix} \\ &= \begin{pmatrix} a_{ij} & a_{ij}p_{ij}^2b_{ij}^*b_{11}v \\ v^*b_{11}^*b_{ij}p_{ij}^2a_{ij} & v^*b_{11}^*b_{ij}p_{ij}^2a_{ij}p_{ij}^2b_{ij}^*b_{11}v + c_{ij} \end{pmatrix} \\ &\stackrel{(\text{A2})}{=} \begin{pmatrix} a_{ij} & (a_{ij}^{\frac{1}{2}}p_{ij})^2b_{ij}^*b_{11}v \\ v^*b_{11}^*b_{ij}(p_{ij}a_{ij}^{\frac{1}{2}})^2 & v^*b_{11}^*b_{ij}p_{ij}a_{ij}^{\frac{1}{2}}p_{ij}^2a_{ij}^{\frac{1}{2}}p_{ij}b_{ij}^*b_{11}v + c_{ij} \end{pmatrix} \\ &\stackrel{(\text{A3})}{=} a'_{ij}. \end{aligned}$$

From $A \in \mathcal{M}^{(3)}$ and (A1) we obtain the condition on the sums for all but the lower right entry. For the lower right entry we first compute

$$\begin{aligned} \left(\sum_{k=1}^3 b_{ik}p_{ik}^2b_{ik}^* \right)^2 &= \sum_{k,l=1}^3 b_{ik}p_{ik}^2b_{ik}^*b_{il}p_{il}^2b_{il}^* \\ &= \sum_{k,l=1}^3 b_{ik}p_{ik}^2(\delta_{kl}a_{ik} - a_{ik}a_{il})p_{il}^2b_{il}^* \\ &\stackrel{(\text{A2})}{=} \left(\sum_{k=1}^3 b_{ik}p_{ik}a_{ik}^{\frac{1}{2}}p_{ik}^2a_{ik}^{\frac{1}{2}}p_{ik}b_{ik}^* \right) - \left(\sum_{k,l=1}^3 b_{ik}(p_{ik}a_{ik}^{\frac{1}{2}})^2(a_{il}^{\frac{1}{2}}p_{il})^2b_{il}^* \right) \\ &\stackrel{(\text{A3})}{=} \left(\sum_{k=1}^3 b_{ik}p_{ik}^2b_{ik}^* \right) - \left(\sum_{k,l=1}^3 b_{ik}b_{il}^* \right) \stackrel{(\text{A1})}{=} \sum_{k=1}^3 b_{ik}p_{ik}^2b_{ik}^*. \end{aligned}$$

It follows that

$$\sum_{k=1}^3 b_{ik} p_{ik}^2 b_{ik}^* \leq I_t.$$

Since $v^* b_{11}^* b_{11} v = 1$, we therefore get

$$\begin{aligned} s_{i*} &:= \sum_{j=1}^3 v^* b_{11}^* b_{ij} p_{ij}^2 b_{ij}^* b_{11} v \leq 1 \\ s_{*j} &:= \sum_{i=1}^3 v^* b_{11}^* b_{ij} p_{ij}^2 b_{ij}^* b_{11} v \leq 1 \\ s &:= \sum_{j=1}^3 (1 - s_{*j}) = \sum_{i=1}^3 (1 - s_{i*}) \geq 0. \end{aligned}$$

So if we choose

$$c_{ij} := \begin{cases} 0 & , \text{ if } s = 0 \\ \frac{(1 - s_{i*})(1 - s_{*j})}{s} & , \text{ else} \end{cases}$$

then we have $c_{ij} \geq 0$ and the condition on the sums is satisfied. □

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DATA AVAILABILITY

The data that supports the findings of this study are available within the article and its supplementary material.

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