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Master's Thesis

Quantum Generalization of Magic Squares and Latin Squares

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Contents

1 Introduction

Quantum theory gives rise to many interesting mathematical objects. It is thus not surprising that concepts which fascinated even medieval mathematicians have been brought to the quantum domain to attract today's researchers. Two such instances are quantum Latin squares and quantum magic squares which are in the focus of this thesis.

Magic squares, squares filled with nonnegative numbers such that the entries in each row and column (and sometimes also the diagonal) sum the same magic constant, fascinate mathematicians and non-mathematicians for more than 2000 years. If the magic constant is one (and there is no condition on the diagonal), they are sometimes also called doubly stochastic matrices. We will use the notions magic square and doubly stochastic matrix interchangeably in this work. Birkhoff-von Neumann's Theorem states that every magic square is in the convex hull of the set of permutation matrices, see Chapter 2.1. We generalize this setting, following the work of Tim Netzer, Gemma De las Cuevas and Tom Drescher [8], by consider a quantum generalization of magic squares and permutation matrices where the entries are no longer numbers, but elements from arbitrary C^*- algebras (Chapter 2.2). In this setting each row and each column of the quantum magic square will form a positive operator valued measure, the most general measure for quantum states. We use a generalization of the convex hull, the matrix convex hull (Chapter 2.3.1), as used in free semialgebraic geometry, and we show that a generalization of Birkhoff-von Neumann's Theorem does not hold: the matrix convex hull of the quantum permutation matrices does not give the full set of quantum magic squares (Theorem 2.41).

Arveson extreme points are a generalization of extreme points to the setting of free spectrahedrons (Chapter 5). The set of quantum magic squares is such a free spectrahedron and the quantum permutation matrices are Arveson extreme points of it, but there must be more Arveson extreme points.
A quantum magic square is called semiclassical if it is in the matrix convex hull of the classical magic squares. We show that the set of semiclassical quantum magic squares is the matrix convex hull of the quantum permutation matrices where all entries commute (Theorem 2.37).

On the other hand, about 300 years ago, Latin squares where introduced, mostly to help with the construction of magic squares. A Latin square is a square of size n filled with the numbers from one to n such that each number appears exactly once in each row and column. A special case of Latin squares of size 9 are known as Sudokus. But Latin squares also have several applications in mathematics, for example in the design of experiments [1] and as multiplication tables of quasigroups [27]. Of course every Latin square is a non-normalized magic square.
Independently of quantum magic squares, a quantum version of Latin squares was introduced by Benjamin Musto and Jamie Vicary in [19]. Instead of num-

bers as entries in the Latin squares, they take quantum states, or from a mathematical perspective, normalized vectors from some $\mathbb{C}^n$. The vectors in each row and column have to form an orthonormal basis. Following [19], we then show that we can use the so called quantum shift-and-multiply method to construct new unitary error bases using quantum Latin squares. Unitary error bases are special bases of $\mathrm{Mat}_n(\mathbb{C})$ that are widely used in quantum information theory [17], the most famous example being the Pauli matrices (Chapter 3).

The main part of this thesis is then to combine the notions of quantum Latin squares and quantum magic squares and investigate the new structures that arise from there (Chapter 4).
We embed quantum Latin squares into the setting of quantum magic squares and give several methods to construct quantum magic squares using classical Latin squares. All the quantum magic squares we construct using Latin squares will be semiclassical. This justifies the notion "semiclassical" even further since this set really captures every quantum magic square that arises from some classical object (Corollary 4.14).
The set of embedded quantum Latin squares is exactly the set of all quantum magic squares where each entry has rank one. One still open question is whether the matrix convex hull of all embedded quantum Latin squares is equal to the convex hull of all quantum permutation matrices. If this would hold it might also have some meaning in the setting of quantum permutation groups.

In Chapter 6, we give a summary of other fields where quantum magic squares appear in one form or another, namely orthogonal quantum Latin squares, SudoQ - a quantum version of Sudokus, quantum permutation groups, and doubly normalized tensors of positive semi-definite operators. We give a short idea of how the concepts could be connected and gain insight from each other.
Lastly, we summarize all the open questions that arose during the work on this thesis in Chapter 7.
In the Appendix, we list basic notations along with further definitions and proofs about convex cones, operator systems and free spectrahedrons.

2 Quantum Magic Squares

2.1 Classical Magic Squares

The oldest know magic square was found in China and dates back to 190 BCE [29]. It is a 3×3 square filled with positive integers satisfying the following rule:
The sum of the numbers in each row, each column and in both main diagonals are the same.
Magic squares, also of different sizes, were afterwards widely studied by mathematicians all around the world. The seemingly 'magic' way in which the numbers added up fascinated even non-mathematicians and magic squares were found in many religious contexts [30]. Historic examples can be seen in Figure 1.

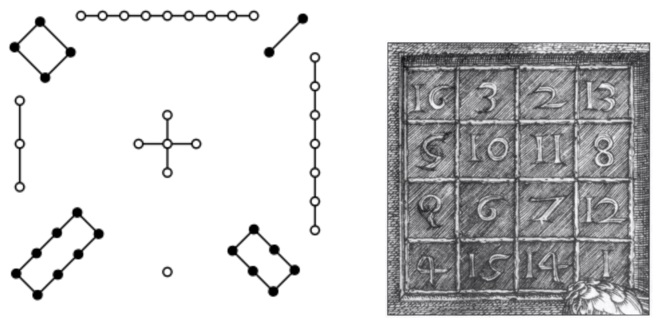

Figure 1: On the left: Chinese Lo Shu Magic Square, the number of dots indicate the number in this 3×3 magic square.
On the right: Abrecht Dürer's Magic Square from his work Melencolia I.

In this work, when we talk about magic squares, we will refer to a somewhat simplified version, sometimes called doubly stochastic matrices:

Definition 2.1. A **magic square** of order $n \in \mathbb{N}$ is a $n \times n$ matrix $A \in \mathrm{Mat}_n(\mathbb{R})$ such that:

- $\forall i, j \in \{1, \ldots, n\}: \ A_{i,j} \in [0,1]$
- $\forall j \in \{1, \ldots, n\}: \ \sum_{i=1}^{n} A_{i,j} = 1$
- $\forall i \in \{1, \ldots, n\}: \ \sum_{j=1}^{n} A_{i,j} = 1$

Remark 2.2.
- In words, we drop the assumption on the diagonals and normalize by the 'magic constant', i.e. the sum of the numbers in each

row and column. This is what we will call a magic square from now on.

- Albrecht Dürer's Magic Square from Figure 2.1 would, in our setting, then become

$$\begin{array}{|c|c|c|c|}\hline \frac{16}{34} & \frac{3}{34} & \frac{2}{34} & \frac{13}{34} \\ \hline \frac{5}{34} & \frac{10}{34} & \frac{11}{34} & \frac{8}{34} \\ \hline \frac{9}{34} & \frac{6}{34} & \frac{7}{34} & \frac{12}{34} \\ \hline \frac{4}{34} & \frac{15}{34} & \frac{14}{34} & \frac{1}{34} \\ \hline \end{array}.$$

- Doubly stochastic matrices, or for us magic squares, appear in different areas of mathematics, for example as transition matrices in special Markov chains [5], [6].

The most famous result about magic squares is the Birkhoff-von Neumann Theorem, which says that the set of magic squares is equal to the convex hull of the permutation matrices.

Definition 2.3. A $n \times n$ **permutation matrix** is a matrix $P \in \mathrm{Mat}_n(\mathbb{C})$ that is obtained by permuting the columns of the identity matrix I_n.
Hence, in reach row and column, there will be exactly one entry equal to 1 and the rest 0.
Given some permutation $\pi \in \mathcal{S}_n$, we will denote the corresponding permutation matrix with $P_\pi \in \mathrm{Mat}_n(\mathbb{C})$. We then have

$$(P_\pi)_{i,j} = \begin{cases} 1 & \text{if } \pi(i) = j \\ 0 & \text{else} \end{cases}$$

Theorem 2.4 (Birkhoff-von Neumann)**.** Given a magic square $A \in \mathrm{Mat}_n(\mathbb{R})$ there exist $k \in \mathbb{N}, \lambda_1, \ldots, \lambda_k \in [0,1]$ with $\sum_{i=1}^k \lambda_i = 1$ and permutation matrices $P_1, \ldots, P_k \in \mathrm{Mat}_n(\mathbb{R})$ such that

$$A = \sum_{i=1}^{k} \lambda_i P_i$$

Proof. Given a magic square A, if we can always find a permutation matrix P such that whenever $P_{i,j} \neq 0$ then $A_{i,j} \neq 0$, we can do the following iteration:
Given A find a corresponding permutation matrix P. Set

$$\lambda = \min\{A_{i,j} | P_{i,j} \neq 0, i, j \in \{1, \ldots, n\}\}$$

Then $A - \lambda P$ is almost a magic square, since $\sum_i (A - \lambda P)_{i,j} = 1 - \lambda$ for each j and similar also for the column sums. Note that if $\lambda = 1$ then $A - \lambda P = 0$ is the zero matrix and hence $A = \lambda P$, we are done. If $\lambda \neq 1$ then $\frac{1}{1-\lambda}(A - \lambda P)$ is a

magic square. But now at least one more entry is equal to zero. So after finitely many iterations, we have found a representation of A as convex combination of permutation matrices.
But how do we find such a permutation matrix?
For that, we will use some basic graph theory. All graphs will be simple graphs without loops.
We will follow the argument from [15]

Definition 2.5. (1) Given a magic square $A \in \mathrm{Mat}_n(\mathbb{R})$ we define its associated graph in the following way: The vertex set is $V = \{r_1, \ldots, r_n, c_1, \ldots, c_n\}$ where r_i represents row i of A and c_j represents column j.
The edge set E is defined by

$$(r_i, c_j) \in E \iff A_{i,j} \neq 0$$

i.e. we connect one row vertex with a column vertex if the entry of A in this row and column is non-zero.
This graph is clearly bipartite.

(2) A **matching** of a graph $G = (V, E)$ is a set $M \subseteq E$ of independent edges, i.e. no two edges in M have the same start or end points.
A matching M is called **perfect** if $|M| = \frac{|V|}{2}$ (it is as large as possible). Note that a perfect matching is only possible if the graph has an even number of vertices.

(3) A matching M **covers** a set $X \subseteq V$ if every $x \in X$ appears in one edge in M.

(4) Given a set $X \subseteq V$, the set of neighbours of X is defined as

$$N(X) := \{v \in V \setminus X \mid \exists x \in X : (x, v) \in E\}$$

Theorem 2.6 (Hall's Marriage Theorem)**.** Given a bipartite graph $G = (V, E)$ with bipartite sets A, B, there exists a matching M which covers A if and only if

$$\forall X \subseteq A: \ |N(X)| \geq |X|$$

The proof of this theorem can be found in Hall's original paper [13], but also in many lecture notes, for example [25].

Lemma 2.7. The associated graph of any magic square has a perfect matching.

Proof. Let $A \in \mathrm{Mat}_n(\mathbb{R})$ be a magic square with associated graph $G = (V, E)$. The graph is bipartite with bipartite sets R, C corresponding to the row and column indices. Assume, for the sake of contradiction, that G has no matching covering R. Then by Hall's Marriage Theorem there exists a set $X \subseteq R$ such that $|N(X)| < |X|$. Note that $N(X) \subseteq C$ represents columns. Thus we can consider the sum

$$\sum_{i \in X, j \in N(X)} A_{i,j} \overset{(*)}{=} \sum_{i \in X} \sum_{j=1}^{n} A_{i,j} = \sum_{i \in X} 1 = |X|.$$

In $(*)$ we use that $A_{i,j} = 0$ if i and j are not connected in G.
On the other hand, since all entries of A are non-negative, we get

$$\sum_{i \in X, j \in N(X)} A_{i,j} \leq \sum_{j \in N(X)} \sum_{i=1}^{n} A_{i,j} = |N(X)| < |X| = \sum_{i \in X, j \in N(X)} A_{i,j}$$

which gives the desired contradiction. $\square$

Now back to the proof of Birkhoff-von Neumann's Theorem.
Will still need to show the following:
Given a magic square A, we can always find a permutation matrix P such that whenever $P_{i,j} \neq 0$ then $A_{i,j} \neq 0$.
By the previous Lemma, the graph $G = (V, E)$ associated to A has a perfect matching M that covers all row indices and hence also all column indices. Now let $P \in \mathrm{Mat}_n(\mathbb{R})$ be the matrix where

$$P_{i,j} = \begin{cases} 1 & \text{if } (i,j) \in M \\ 0 & \text{else} \end{cases}$$

Then P is a permutation matrix, since exactly one entry in each row and column will be equal to 1 and the rest 0.
Furthermore, we get that if $P_{i,j} \neq 0$ then $(i,j) \in E$ which is equivalent to $A_{i,j} \neq 0$.
Thus the matrix P is exactly what we were looking for.

$\square$

Following [4], we will examine the extreme points of the set of magic squares.

Definition 2.8. Given a vector space V and a subset $A \subseteq V$, a point $u \in A$ is called *extreme point* if whenever there are $v, w \in A$ such that $u = \frac{v+w}{2}$ then $u = v = w$.

Note that for a convex set A this definition is equivalent to saying that $u \in A$ is an extreme point if whenever $u = \lambda v + (1-\lambda)w$ for some $\lambda \in (0, \frac{1}{2}], v, w \in A$ then $u = v = w$, because

$$u = \lambda v + (1-\lambda)w = \frac{1}{2}(2\lambda v + (1-2\lambda)w) + \frac{1}{2}w$$

and $2\lambda v + (1-2\lambda)w \in A$.

Proposition 2.9. The $n \times n$ permutation matrices are the extreme points of the so called Birkhoff polytop: the set of $n \times n$ magic squares.

Proof. Assume we have a $n \times n$ permutation matrix P that can be written as $P = \frac{1}{2}(V + W)$ where V, W are magic squares.
Whenever $P_{i,j} = 0$ then also $V_{i,j} = W_{i,j} = 0$ since all entries of V and W are non-negative. But then $P = V = W$ has to hold.

On the other hand, if a magic square X is an extreme point, by Birkhoff-von Neumann's Theorem (2.4) it can be written as a convex combination of permutation matrices:

$$X = \sum_{i=1}^{t} \lambda_i P_i$$

Without loss of generality, we can assume that $\lambda_1 = \min\{\lambda_i \mid i = 1, \dots, t\}$ Hence, $\frac{\lambda_i}{1-\lambda_1} \leq 1$ for all $i \geq 2$ and since the set of magic squares is convex and $1 - \lambda_1 = \sum_{i=2}^{t} \lambda_i$ we get that $Q := \sum_{i=2}^{t} \frac{\lambda_i}{1-\lambda_1} P_i$ is again a magic square. Then, since X is an extreme point,

$$X = \lambda_1 P_1 + (1 - \lambda_1) Q$$

implies that $X = P_1$ is a permutation matrix. □

2.2 Quantum Version

In this section, we want to generalize the notion of magic squares. Instead of numbers, we will use matrices as the entries of the magic square. What rules should the matrices follow?
In an $n \times n$ magic square, each row and each column forms a probability distribution on the numbers $\{1, \dots, n\}$. In the language of quantum physics, the analogues notion is a positive operator valued measure, or short POVM.

Definition 2.10. A positive operator valued measure is a set of n matrices $P_1, \dots, P_n \in \mathrm{Her}_s(\mathbb{C})$ such that each P_i is positive semi-definite ($P_i \geq 0$) and

$$\sum_{i=1}^{n} P_i = \mathrm{I}_s$$

Following this generalization of a measure on numbers to a measure on quantum states, we get to our definition of quantum magic squares:

Definition 2.11. A quantum magic square (QMS) of interior size s and exterior size n is a matrix $A \in \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C}))$ such that each row and each column of A forms a POVM. Or more detailed, A has to satisfy:

- $\forall\ i, j \in \{1, \dots, n\} : A_{i,j} \geq 0$
- $\forall\ i \in \{1, \dots, n\} : \sum_{j=1}^{n} A_{i,j} = \mathrm{I}_s$
- $\forall\ j \in \{1, \dots, n\} : \sum_{i=1}^{n} A_{i,j} = \mathrm{I}_s$

Example 2.12. Below is an example of a quantum magic square of exterior size 3 and interior size 2.

$\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 \\ 0 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & 0 \\ 0 & 0 \end{pmatrix}$
$\begin{pmatrix} 1/4 & 1/8 \\ 1/8 & 1/4 \end{pmatrix}$	$\begin{pmatrix} 3/4 & -1/8 \\ -1/8 & 1/4 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 \\ 0 & 1/2 \end{pmatrix}$
$\begin{pmatrix} 1/4 & -1/8 \\ -1/8 & 1/4 \end{pmatrix}$	$\begin{pmatrix} 1/4 & 1/8 \\ 1/8 & 1/4 \end{pmatrix}$	$\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$

Remark 2.13. (1) We can generalize this notion even further by allowing the entries of A to be positive elements in any C^*-algebra such that each row and column sum to the identity element of the algebra. But we will not consider this case any further in this work, since at least every finite dimensional C^*-algebra is covered by the matrix case.

(2) Every quantum magic square with interior size 1 is a magic square.

(3) For exterior size $n = 1$ the only possible QMS is

$$A = (\mathrm{I}_s)$$

(4) For $n = 2$ all QMS have the form

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

where $a, \mathrm{I}_s - a \in \mathrm{Her}_s(\mathbb{C})$ are positive semi-definite.

2.2.1 Different Types

From now on, we will fix the exterior size $n \in \mathbb{N}$ of the quantum magic square.

In this section, we will define a generalization of permutation matrices and two other types of quantum magic squares: semiclassical quantum magic squares and commuting quantum permutation matrices. Here, we follow [8].

Definition 2.14. Let $A = (A_{i,j})_{i,j=1}^n \in \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C}))$ be a quantum magic square. Then A is called

- **quantum permutation matrix** if all $A_{i,j} \in \mathrm{Her}_s(\mathbb{C})$ are projectors, i.e. $A_{i,j}^2 = A_{i,j}$

- **quantum commuting permutation matrix** if A is a quantum permutation matrix and all $A_{i,j}$ commute, i.e. $A_{i,j}A_{\ell,k} = A_{\ell,k}A_{i,j}$ for all $i, j, \ell, k \in \{1, \dots, n\}$.

- **semiclassical** if there exist permutation matrices $P_\pi \in \mathrm{Mat}_n(\mathbb{C})$ and positive semi-definite matrices $q_\pi \in \mathrm{Her}_s(\mathbb{C})$ for each $\pi \in S_n$ with $\sum_{\pi \in S_n} q_\pi = \mathrm{I}_s$ such that
$$A = \sum_{\pi \in S_n} P_\pi \otimes q_\pi.$$
S_n denotes the set of permutations of n elements.

Remark 2.15. (1) A quantum permutation matrix with interior size 1 is permutation matrix in the classical sense, since the only projectors in $\mathbb{C}$ are 0 and 1 and the magic square condition makes sure that there is exactly one 1 entry in each row and column.

(2) Every magic square is a semiclassical quantum magic square with interior size 1, by Birkhoff-von Neumanns Theorem (2.4).

(3) Every quantum magic square of exterior size $n = 1, 2$ is semiclassical. This follows from the argument in Remark 2.13 (4), since we know how all possible such QMS look like.

Proposition 2.16. Every quantum permutation matrix $A \in \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C}))$ is a unitary in the sense that $A^*A = AA^* = \mathrm{I}_{n \cdot s}$

Proof. From the magic square condition, we get that for all $i, j \in \{1, \dots, n\}$:
$$\sum_{\ell=1}^{n} A_{i,\ell} = \sum_{\ell=1}^{n} A_{\ell,j} = \mathrm{I}_s$$
On the other hand, the entries of A are projectors, hence $A_{i,j}A_{i,k} = 0$ for $j \neq k$ because
$$\begin{aligned} A_{i,k} &= \left(\sum_j A_{i,j}\right) A_{i,k} = A_{i,k} + \sum_{j \neq k} A_{i,j}A_{i,k} \\ &\Rightarrow \sum_{j\neq k} A_{i,j}A_{i,k} = 0 \\ &\overset{A_{i,j}A_{i,k}\geq 0}{\Rightarrow} \forall j \neq k: \ A_{i,j}A_{i,k} = 0 \end{aligned}$$
An analogous argument also shows $A_{j,i}A_{k,i} = 0$ for $j \neq k$.
Hence
$$(AA^*)_{i,j} = \sum_k A_{i,k}A_{j,k}^* \overset{A_{j,k}\in \mathrm{Her}_s(\mathbb{C})}{=} \delta_{i,j} \sum_k A_{i,k}A_{i,k} \overset{A_{i,k}^2 = A_{i,k}}{=} \delta_{i,j} \sum_k A_{i,k} = \delta_{i,j}\, \mathrm{I}_s$$
And similar for A^*A □

Definition 2.17. We use the following notation for $n, s \in \mathbb{N}$:

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

and

$$
\mathcal{M}^{(n)} := \bigcup_{s\in\mathbb{N}} \mathcal{M}_s^{(n)} \qquad \mathcal{P}^{(n)} := \bigcup_{s\in\mathbb{N}} \mathcal{P}_s^{(n)} \qquad \mathcal{CP}^{(n)} := \bigcup_{s\in\mathbb{N}} \mathcal{CP}_s^{(n)} \qquad \mathcal{SC}(n) = \bigcup_{s\in\mathbb{N}} \mathcal{SC}_s^{(n)}.
$$

Remark 2.18. It directly follows that we have the following inclusions:

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

For exterior size $n = 1, 2, 3$ we have

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

For $n = 1, 2$ we know the form of each quantum magic square (see Remark 2.13) and there we can see that the entries of each quantum permutation matrix automatically commute.
A proof for the case $n = 3$ can be found in [18].
For $n \geq 4$ we have $\mathcal{CP}^{(n)} \subsetneq \mathcal{P}^{(n)}$ which can be seen by taking block diagonal sums of quantum permutation matrices. For more details see the example in the proof of Proposition 2.21.

2.3 Background from Semialgebraic Geometry and Operator Algebra

Non-commutative or free semialgebraic geometry is a generalization of semialgebraic geometry, the study of sets of real solutions of polynomial equalities or inequalities. For example, given a polynomial $p \in \mathbb{R}[x]$ then $\{t \in \mathbb{R} \mid p(t) \geq 0\}$ would be a set that is studied in semialgebraic geometry, while $\{M \in \mathrm{Her}_s(\mathbb{C}) \mid s \in \mathbb{N},\ p(M) \geq 0 \text{ i.e. } p(M) \text{ is psd}\}$ would be the analogues free semialgebraic set. This can then be generalized to (non-commutative) polynomials in several variables.
Some definitions and results from this field will be interesting for us.

2.3.1 Matrix Convex Hull

We start with the definition of a free set following [14] and we will see that the sets in Definition 2.17 will fit this concept. Then, we will generalize the notion of convexity to fit the properties of free sets.

Definition 2.19. Let $F_s \subseteq \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C}))$ for all $s \in \mathbb{N}$ and $F = \bigcup_{s\in\mathbb{N}} F_s$. Then F is called a **free set** if

(1) it is closed with respect to direct sums, i.e. given $A = (A_{i,j})_{i,j=1}^n \in F_s,\ B = (B_{i,j})_{i,j=1}^n \in F_k$ then

$$A \oplus B := \left(\begin{pmatrix} A_{i,j} & 0 \\ 0 & B_{i,j} \end{pmatrix} \right)_{i,j=1}^n \in F_{s+k}.$$

(2) it is closed with respect to simultaneous unitary conjugation, i.e. for each $s \in \mathbb{N}$, each $A \in F_s$ and each unitary $U \in \mathrm{Mat}_s(\mathbb{C})$ we have

$$U^*AU := (U^*A_{i,j}U)_{i,j=1}^n \in F_s$$

Note: the set F_s is called the s-th level of F.

Remark 2.20. The above definition varies from the standard definition. Usually, one would consider n-tuples of hermitian matrices, i.e. $F_s \subseteq (\mathrm{Her}_s(\mathbb{C}))^n$, since this is more natural when you want to plug the matrices into a multivariate polynomial. But since tuples and matrices are the same up to rearranging, as long as one does not multiply, we did not really change the definition. The same also holds for the upcoming definition of matrix convexity 2.23.

Proposition 2.21. The sets $\mathcal{M}^{(n)}, \mathcal{P}^{(n)}, \mathcal{CP}^{(n)}$ and $\mathcal{SC}^{(n)}$ are free sets.

Proof. Let $A, B \in \mathcal{M}^{(n)}$ then $A \oplus B \in \mathcal{M}^{(n)}$ since the sum over the entries of each row and column is still the identity.
Let $A \in \mathcal{M}_s^{(n)}, U \in \mathrm{Mat}_s(\mathbb{C})$ unitary, then all entries of U^*AU will be psd since conjugation does not change this property. And we have for the i-th row

$$\sum_j U^*A_{i,j}U = U^* \left(\sum_j A_{i,j} \right) U = U^*U = \mathrm{I}_s$$

and similar for the columns, hence $U^*AU \in \mathcal{M}^{(n)}$.
For $A, B \in \mathcal{P}^{(n)}$ we have $A \oplus B \in \mathcal{P}^{(n)}$, since

$$(A \oplus B)_{i,j}^2 = \begin{pmatrix} A_{i,j}^2 & 0 \\ 0 & B_{i,j}^2 \end{pmatrix} = \begin{pmatrix} A_{i,j} & 0 \\ 0 & B_{i,j} \end{pmatrix} = (A \oplus B)_{i,j}.$$

If $A \in \mathcal{P}^{(n)}$ then $A_{i,j}$ is a projector and so is $U^*A_{i,j}U$ since $(U^*A_{i,j}U)(U^*A_{i,j}U) = U^*A_{i,j}^2U = U^*A_{i,j}U$. Hence $U^*AU \in \mathcal{P}^{(n)}$.
$\mathcal{CP}^{(n)}$ is also closed under unitary conjugation, since we use the same matrix to conjugate every entry, hence these entries still commute.
Given $A, B \in \mathcal{CP}^{(n)}$. Then for arbitrary $i, j, k, \ell \in \{1, \dots, n\}$ we have

$$\begin{aligned}(A \oplus B)_{i,j}(A \oplus B)_{k,\ell} &= \begin{pmatrix} A_{i,j} & 0 \\ 0 & B_{i,j} \end{pmatrix} \begin{pmatrix} A_{k,\ell} & 0 \\ 0 & B_{k,\ell} \end{pmatrix} = \begin{pmatrix} A_{i,j}A_{k,\ell} & 0 \\ 0 & B_{i,j}B_{k,\ell} \end{pmatrix} \\ &\overset{A,B\in\mathcal{CP}^{(n)}}{=} \begin{pmatrix} A_{k,\ell}A_{i,j} & 0 \\ 0 & B_{k,\ell}B_{i,j} \end{pmatrix} = (A \oplus B)_{k,\ell}(A \oplus B)_{i,j}.\end{aligned}$$

Hence $A \oplus B \in \mathcal{CP}^{(n)}$.

Given $A = \sum_\pi P_\pi \otimes q_\pi \in \mathcal{SC}^{(n)}$ then $U^*AU = \sum_\pi P_\pi \otimes U^* q_\pi U \in \mathcal{SC}^{(n)}$. Let $A = \sum_\pi P_\pi \otimes a_\pi, B = \sum_\pi P_\pi \otimes b_\pi \in \mathcal{SC}^{(n)}$. Then

$$(A \oplus B)_{i,j} = \sum_{\pi \in S_n:\ \pi(i)=j} \begin{pmatrix} a_\pi & 0 \\ 0 & b_\pi \end{pmatrix} = \left(\sum_{\pi \in \mathcal{S}_n} P_\pi \otimes \begin{pmatrix} a_\pi & 0 \\ 0 & b_\pi \end{pmatrix} \right)_{i,j}$$

and therefore $A \oplus B \in \mathcal{SC}^{(n)}$.

$\square$

Next, let us recall the definition of a convex set in order to generalize to our free setting later.

Definition 2.22. Let V be a $\mathbb{R}$ or $\mathbb{C}$ vector space. Then a set $A \subseteq V$ is called convex it for all $n \in \mathbb{N}, a_1, \ldots, a_n \in A$ and all scalars $\lambda_1, \ldots, \lambda_n \geq 0$ with $\sum_i \lambda_i = 1$ we have

$$\sum_{i=1}^n \lambda_i a_i \in A$$

Every level $\mathcal{M}_s^{(n)}$ is convex. This is not true for $\mathcal{P}^{(n)}$ and $\mathcal{CP}^{(n)}$ since the convex combination of projectors is not necessarily a projector. But each level of $\mathcal{SC}^{(n)}$ is convex which will follow from Proposition 2.25.
But the concept of level-wise convexity is not enough in our setting, since we have the possibility to connect different layers. This should be reflected in the notion of convexity that we use. Hence the following definition:

Definition 2.23. Let for every $s \in \mathbb{N}$ some $R_s \subseteq \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C}))$ be given. Then $R = \bigcup_{s \in \mathbb{N}} R_s$ is called **matrix convex** if for all $r, s_i, t \geq 1, A^{(i)} \in R_{s_i}$ for $i = 1, \ldots, r$ and $V_i \in \mathrm{Mat}_{s_i,t}(\mathbb{C})$ with $\sum_i V_i^* V_i = \mathrm{I}_t$ we have

$$\left(\sum_{i=1}^r V_i^* A_{\ell,k}^{(i)} V_i \right)_{\ell,k=1}^n \in R_t$$

mconv(R) denotes the smallest matrix convex superset of R.

Remark 2.24. (1) The intersection of matrix convex sets is matrix convex, therefore the matrix convex hull always exists. For example given some set $R = \bigcup_{s \in \mathbb{N}} R_s$ like above, which is closed under direct sums, we have

$$mconv(R) = \bigcup_{s \in \mathbb{N}} \{A \in \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C})) \mid \exists V \in \mathrm{Mat}_{m,s}(\mathbb{C}) \text{ isometry }, Z \in R_m :\ A = V^* Z V\}$$

see [14] Chapter 2.4 for more details.

(2) If a set is matrix convex, then each level is convex in the standard sense. Given $\lambda_1, \lambda_2 \in [0,1]$ with $\lambda_1 + \lambda_2 = 1$ set $V_1 = \sqrt{\lambda_1}\,\mathrm{I}_s, V_2 = \sqrt{\lambda_2}\,\mathrm{I}_s$ and let $A^{(1)}, A^{(2)} \in R_s$. Then the matrix convexity of R implies that

$$V_1^* A^{(1)} V_1 + V_2^* A^{(2)} V_2 = \lambda_1 A^{(1)} + \lambda_2 A^{(2)} \in R_s.$$

But the converse implication is not true.

(3) The set of quantum magic squares $\mathcal{M}^{(n)}$ is matrix convex. To see this, let, for $i = 1, \ldots, r:\ A^{(i)} \in \mathcal{M}_{s_i}^{(n)}, V_i \in \mathrm{Mat}_{s_i,t}(\mathbb{C})$ with $\sum_i V_i^* V_i = \mathrm{I}_t$. We want to show:

$$\left(\sum_{i=1}^{r} V_i^* A_{\ell,k}^{(i)} V_i\right)_{\ell,k=1}^{n} \in \mathcal{M}_t^{(n)}$$

Fix a row ℓ. Then the sum over the elements in this row is

$$\sum_{k=1}^{n}\sum_{i=1}^{r} V_i^* A_{\ell,k}^{(i)} V_i = \sum_{i=1}^{r} V_i^* \left(\sum_{k=1}^{n} A_{\ell,k}^{(i)}\right) V_i = \sum_{i=1}^{r} V_i^*\, \mathrm{I}_{s_i}\, V_i = \mathrm{I}_t\,.$$

Hence, each row sums to the identity and a similar calculation shows the same for the columns. Furthermore, the sum and conjugate of positive semi-definite matrices is again positive semi-definite, hence B is indeed a quantum magic square.

(4) For $n \geq 2$ the sets $\mathcal{CP}^{(n)}$ and $\mathcal{P}^{(n)}$ are not matrix convex. This follows from the fact that convex combinations of projectors are not necessarily projectors again.
We get the following inclusions:

$$mconv\left(\mathcal{CP}^{(n)}\right) \subseteq mconv\left(\mathcal{P}^{(n)}\right) \subseteq \mathcal{M}^{(n)}$$

From Remark 2.13 we can see that for $n \leq 2$ all inclusions are equalities. For $n = 3$ the left inclusion is an equality by Remark 2.18. We will later in Theorem 2.41 see that the inclusion on the right is not an equality for $n \geq 3$.

Proposition 2.25. The set of semiclassical quantum magic squares is the matrix convex hull of the classical magic squares, and hence, by Birkhoff-von Neumanns Theorem (2.4), the matrix convex hull of the classical permutation matrices.
Or expressed in formulas:

$$\mathcal{SC}^{(n)} = mconv(\mathcal{M}_1^{(n)}) = mconv(\mathcal{P}_1^{(n)})$$

Proof. Let $A = \sum_{\pi \in S_n} P_\pi \otimes q_\pi \in \mathcal{SC}_t^{(n)}$ be a semiclassical QMS. Then, by definition, each $q_\pi \geq 0$. Therefore it can be written as a square of a matrix

$V_\pi \in \mathrm{Mat}_t(\mathbb{C}) : q_\pi = V_\pi^* V_\pi$. Hence,

$$A_{\ell,k} = \left(\sum_\pi P_\pi \otimes V_\pi^* V_\pi \right)_{\ell,k} = \sum_\pi (P_\pi)_{\ell,k} V_\pi^* V_\pi = \sum_\pi V_\pi^* (P_\pi)_{\ell,k} V_\pi.$$

And we have $\sum_\pi V_\pi^* V_\pi = \sum_\pi q_\pi = \mathrm{I}_t$. Therefore, $A \in mconv(\mathcal{P}_1^{(n)})$.
The other direction follows in the same manner, just do the above calculations backwards. ☐

This proposition shows why the name 'semiclassical' is well chosen, since these are all quantum magic squares that directly arise from classical magic squares using the tool of the matrix convex hull.

2.3.2 Operator Systems

Abstract Operator systems are a structure that come from the study of C^*-algebras. Their structure is similar to the one of free sets with different levels of interior sizes of matrices.
The original definition is quite abstract, we will only need a simplified and adapted version, but we will state it for the sake of completeness. The definitions in this chapter are taken from [10], where more results about abstract operator systems can be found.

Definition 2.26 (Abstract Operator System, original version)**.** Let $\mathcal{V}$ be a $\mathbb{C}$-vector space with involution $*$, $\mathcal{V}_{her} := \{v \in \mathcal{V} \mid v^* = v\}$ the $\mathbb{R}$-subspace of hermitian elements. Then, for any $s \in \mathbb{N}$, we have a canonical involution on $\mathrm{Mat}_s(\mathcal{V}) = \mathcal{V} \otimes \mathrm{Mat}_s(\mathbb{C})$ given by $(v_{i,j})_{i,j}^* = (v_{j,i}^*)_{i,j}$.
An **abstract operator system** $\mathcal{C}$ on $\mathcal{V}$ consists of salient convex cones $\mathcal{C}_s \subseteq \mathrm{Mat}_s(\mathcal{V})_{her}$ for each $s \in \mathbb{N}$, such that

(1) $\forall s, t \in \mathbb{N}, A \in \mathcal{C}_s, V \in \mathrm{Mat}_{s,t}(\mathbb{C}) :\ V^*AV \in \mathcal{C}_t$

(2) $\exists u \in \mathcal{C}_1 \subseteq \mathcal{V}_{her}$ such that

 (a) $\forall s \in \mathbb{N}\ \forall x \in \mathrm{Mat}_s(\mathcal{V})_{her}\ \exists r > 0 :\ r(u \otimes \mathrm{I}_s) + x \in \mathcal{C}_s$

 (b) $\forall s \in \mathbb{N} :$ if $\forall r > 0 : r(u \otimes \mathrm{I}_s) + x \in \mathcal{C}_s$ then $x \in \mathcal{C}_s$

Remark 2.27. (1) Condition (2a) means there has to exist a matrix order unit. This is equivalent to saying that $u \otimes I_s$ is an interior point of $\mathcal{C}_s$ when taking the finest locally convex topology on $\mathcal{V}$.

(2) Condition (2b) says that u has to be an archimedian matrix order unit. This also has an equivalent topological meaning, namely that all $\mathcal{C}_s$ are closed.

(3) There is also the notion of concrete operator system, which is a $*$-subspace of a C^*-algebra containing the one element. The Choi-Effros Theorem states that every abstract operator system is isomorphic (with a certain

construction) to a concrete operator system. But we will not go into details here.
For easier notation, we will drop the 'abstract' from now on since all operator systems that we consider will be of this type.

To use the notion of operator system in the context of quantum magic squares, we need to define a fitting $\mathbb{C}$-vector space $\mathcal{V}$ and look at convex cones in there. The set of quantum magic squares itself can not be an operator system, since the normalization condition bounds the convex sets on each level, they do not form cones. Hence we have to drop the normalization for now, which leads to the following definition that was first formulated in [8].

Definition 2.28. Let $\mathcal{V}^{(n)} = \{A \in \mathrm{Mat}_n(\mathbb{C}) \mid \exists c \in \mathbb{C} : \forall i,j \in \{1,\dots,n\} : \sum_k A_{i,k} = \sum_k A_{k,j} = c\} \subseteq \mathrm{Mat}_n(\mathbb{C})$ be the space of matrices with constant row and column sums. Equip this space with entrywise conjugation as involution. The **magic cone** is the set

$$\mathcal{C}^{(n)} = \{A \in \mathcal{V}^{(n)} \mid \forall i,j : A_{i,j} \in \mathbb{R}_{\geq 0}\} \subseteq \mathcal{V}^{(n)}_{her}.$$

The magic cone is precisely the cone of magic squares in the non-normalized sense.

Let us consider some (classical) geometric properties of these sets, following [8].

Lemma 2.29. (1) $\mathcal{V}^{(n)} = \mathrm{span}_{\mathbb{C}}(\mathcal{P}_1^{(n)})$

(2) $\mathcal{V}^{(n)}_{her} = \mathrm{span}_{\mathbb{R}}(\mathcal{P}_1^{(n)})$

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

(4) $\mathcal{C}^{(n)}$ is a salient polyhedral cone and the all one matrix is an interior point/order unit.

(5) The extreme rays of $\mathcal{C}^{(n)}$ are precisely the ones spanned by the permutation matrices, hence there are $n!$ many.
For $n \geq 3$ $\mathcal{C}^{(n)}$ has n^2 facets, namely $F_{i,j} = \{A \in \mathcal{C}^{(n)} \mid A_{i,j} = 0\}$ for $i,j \in \{1,\dots,n\}$.
In the case $n \geq 3$, $\mathcal{C}^{(n)}$ is not a simplex cone, i.e. the number of extreme rays exceeds its dimension.

Proof. To show the '$\subseteq$' part for (1) and (2) we will consider three cases:

Case 1: $A \in \mathcal{V}^{(n)}_{her}$ and $A_{i,j} \geq 0$ for all i,j (in other words $A \in \mathcal{C}^{(n)}$).
Set $c = \sum_{i=1}^n A_{i,j}$ for some $j \in \{1,\dots,n\}$ the value of the row and column sums, the so called magic constant. Note that if $c = 0$ then $A = 0$ the all zero matrix which is clearly in $\mathrm{span}_{\mathbb{R}}(\mathcal{P}_1^{(n)})$. If $c \neq 0$ then $\frac{1}{c}A$ is a magic square and by Birkhoff-von Neumann's Theorem (2.4) we know $\frac{1}{c}A \in \mathrm{span}_{\mathbb{R}}(\mathcal{P}_1^{(n)})$, hence $A \in \mathrm{span}_{\mathbb{R}}(\mathcal{P}_1^{(n)})$.

Case 2: $A \in \mathcal{V}_{her}^{(n)}$ and there exist some i, j such that $A_{i,j} < 0$.
Let J denote the all one $n \times n$ matrix. Note that $J \in \mathcal{V}_{her}^{(n)}$ with only non-negative entries, hence $J \in \mathrm{span}_{\mathbb{R}}(\mathcal{P}_1^{(n)})$ by the argument in the first case.
Set $m = \max\{|A_{i,j}| \mid A_{i,j} < 0, i, j \in \{1, \ldots, n\}\}$ the absolute value of the smallest entry of A. Then $A + mJ \in \mathcal{V}_{her}^{(n)}$ has per construction only non-negative entries and is, again by case one, in the span of the permutation matrices. But then so is A.
Case 3: $A \in \mathcal{V}^{(n)} \setminus \mathcal{V}_{her}^{(n)}$.
Then $A = \mathrm{Re}(A) + i\,\mathrm{Im}(A)$ where $\mathrm{Re}(A), \mathrm{Im}(A)$ are just the entrywise real an imaginary part. Let $c = c_1 + ic_2$ be the magic constant. For any $j \in \{1, \ldots, n\}$ we get

$$\sum_k A_{k,j} = \sum_k \mathrm{Re}(A_{k,j}) + i \sum_k \mathrm{Im}(A_{k,j}) = c_1 + ic_2$$

Hence,

$$\sum_k \mathrm{Re}(A_{k,j}) = c_1, \ \sum_k \mathrm{Im}(A_{k,j}) = c_2$$

for any j and similarly also for the row sums. Therefore, $\mathrm{Re}(A), \mathrm{Im}(A) \in \mathcal{V}_{her}^{(n)}$ and by case 2, we get $A \in \mathrm{span}_{\mathbb{C}}(\mathcal{P}_1^{(n)})$

For the '$\supseteq$' inclusion, observe that $\mathcal{V}^{(n)}$ ($\mathcal{V}_{her}^{(n)}$) is indeed a $\mathbb{C}$ ($\mathbb{R}$)-vector space: The sum of matrices with constant row and columns sums has again constant row and column sums and the same holds for scalar multiples. Furthermore, we know that every $n \times n$ permutation matrix is in $\mathcal{V}_{her}^{(n)} \subset \mathcal{V}^{(n)}$ and therefore their $\mathbb{C}$ ($\mathbb{R}$)-span has to be contained as well.

Proof of (3):
To get a matrix in $\mathcal{V}^{(n)}$ ($\mathcal{V}_{her}^{(n)}$), we can choose the upper left $n-1 \times n-1$ matrix freely over $\mathbb{C}$ ($\mathbb{R}$), this gives $(n-1)^2$ degrees of freedom.
Next, we can choose the magic constant $c \in \mathbb{C}$ ($c \in \mathbb{R}$), another degree of freedom.
The entries in the n-th row and column have to be chosen in such a way that the rows and columns indeed sum to c. For example $A_{1,n} = c - \sum_{j=1}^{n-1} A_{1,j}$ and

$$A_{n,n} = c - \sum_{j=1}^{n-1} A_{j,n} = c - (n-1)c + \sum_{k,j=1}^{n-1} A_{j,k} = c - \sum_{k=1}^{n-1} A_{n,k}.$$

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

Proof of (4):

- **Cone**:
  Let $\lambda_1, \lambda_2 \in \mathbb{R}_{\geq 0}, A, B \in \mathcal{C}^{(n)}$. Then $(\lambda_1 A + \lambda_2 B)_{i,j} \geq 0$ and $\lambda_1 A + \lambda_2 B \in \mathcal{V}_{her}^{(n)}$ since it is a vector space.

- **Salient**:
$-\mathcal{C}^{(n)} = \{A \in \mathcal{V}_{her}^{(n)} \mid A_{i,j} \leq 0 \ \forall i,j\}$ and therefore $\mathcal{C}^{(n)} \cap -\mathcal{C}^{(n)} = \{0\}$

- **Polyhedral**:
From part (1) case 1 we can see that

$$\mathcal{C}^{(n)} = \mathrm{co}(\mathcal{P}_1^{(n)}) := \left\{ \sum_k \lambda_k P_k \mid \lambda_k \geq 0, P_k \in \mathcal{P}_1^{(n)} \right\}.$$

This means that $\mathcal{C}^{(n)}$ is the conic hull of finitely many elements which is one of the possible (equivalent) ways to define a polyhedral cone.

- **J is interior point/order unit**:
Given some $A \in \mathcal{V}_{her}^{(n)}$, we have already seen in part (1) case 1 that we can find an $m > 0$ such that $mJ + A \in \mathcal{C}(n)$, which is precisely what we needed to show.

Proof of part (5):
First, we show that the rays generated by permutation matrices are indeed extreme rays.
Pick a permutation matrix $P \in \mathcal{P}_1^{(n)}$ and assume there are $A, B \in \mathcal{C}^{(n)}, A, B \neq 0$ such that $\frac{A+B}{2} \in \mathrm{co}(P)$, i.e. there exists a $\lambda \in \mathbb{R}_{\geq 0}$ such that $\frac{A+B}{2} = \lambda P$.
If $P_{i,j} = 0$ then $(A+B)_{i,j} = 0$ and, since $A, B \in \mathcal{C}^{(n)}$, $A_{i,j} = B_{i,j} = 0$. Hence all but one entry in each row and column of A and B are zero. But A, B are non-zero and have constant row and column sums. Therefore they have to be a multiple of P.
On the other hand, any extreme ray of $\mathcal{C}^{(n)}$ has to be generated by a permutation matrix, since $\mathcal{C}^{(n)} = \mathrm{co}(\mathcal{P}_1^{(n)})$.

Lastly, we need to show that for $n \geq 3$ the $F_{i,j} = \{A \in \mathcal{C}^{(n)} \mid A_{i,j} = 0\}$ for $i, j \in \{1, \ldots, n\}$ are the facets of $\mathcal{C}^{(n)}$.
Fix some $i, j \in \{1, \ldots, n\}$. Clearly, $F_{i,j}$ is convex. Assume there are $A, B \in \mathcal{C}^{(n)}$ and $\lambda \in (0,1)$ such that $\lambda A + (1-\lambda) B \in F_{i,j}$. Then $\lambda A_{i,j} + (1-\lambda) B_{i,j} = 0$ and $A_{i,j}, B_{i,j} \geq 0$, hence $A_{i,j} = B_{i,j} = 0$ and therefore $A, B \in F_{i,j}$. Thus, $F_{i,j}$ is face and it has one dimension less then $\mathcal{C}^{(n)}$ since we have one extra restriction.
On the other hand, assume that there is a facet F of $\mathcal{C}^{(n)}$ which is not of the form of any of the $F_{i,j}$. Then for every i, j there exists some $A \in F$ with $A_{i,j} > 0$. Taking a convex combination of all these gives some $B \in F$ such that all entries of B are strictly greater than zero. Now, since $\dim(F) < \dim(\mathcal{C}^{(n)})$ there exists a nonzero $C \in \mathcal{C}^{(n)} \setminus F$. Since $B_{i,j} > 0$ for any i, j we can find a small enough $\varepsilon > 0$ such that $B + \varepsilon C \in \mathcal{C}^{(n)}$ and $B - \varepsilon C \in C^{(n)}$. Both can, due to the limited dimension of F, not be in F. But $\frac{1}{2}(B + \varepsilon C) + \frac{1}{2}(B - \varepsilon C) = B \in F$, a contradiction to F being a facet. $\square$

Now we can consider the for us relevant operator systems over the $\mathbb{C}$-vector space of matrices with constant row and column sums $\mathcal{V}^{(n)} \subseteq \mathrm{Mat}_n(\mathbb{C})$. Keep in mind that we use entrywise conjugation in $\mathcal{V}^{(n)}$, hence $\mathcal{V}^{(n)}_{her} \subseteq \mathrm{Mat}_n(\mathbb{R})$. We will use that $\mathrm{Mat}_n(\mathbb{C}) \otimes \mathrm{Mat}_s(\mathbb{C}) \cong \mathrm{Mat}_n((\mathrm{Mat}_s(\mathbb{C}))$, hence we can consider $\mathcal{V}^{(n)} \otimes \mathrm{Mat}_s(\mathbb{C}) \subseteq \mathrm{Mat}_n((\mathrm{Mat}_s(\mathbb{C}))$ and $(\mathcal{V}^{(n)} \otimes \mathrm{Mat}_s(\mathbb{C}))_{her} \subseteq \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C}))$. In this way we get the structure that we are used to from the quantum magic squares.

Definition 2.30 (Operator System over $\mathcal{V}^{(n)}$)**.** An operator system over $\mathcal{V}^{(n)}$ is a set of non-empty closed salient convex cones $C = \bigcup_{s \in \mathbb{N}} C_s$ with

(1) $\forall s \in \mathbb{N} : C_s \subseteq (\mathcal{V}^{(n)} \otimes \mathrm{Mat}_s(\mathbb{C}))_{her}$

(2) $\forall r, s \in \mathbb{N}\ \forall V \in \mathrm{Mat}_{r,s}(\mathbb{C})\ \forall (A_{i,j})_{i,j} \in C_r :\ (V^* A_{i,j} V)_{i,j} \in C_s$

Next, we will define the minimal and maximal magic operator system. This will be the minimal and maximal operator systems as it is used in free algebraic geometry (for example [10]) over the magic cone.

Definition 2.31 (Minimal Magic Operator System)**.** Let $\mathcal{C}^{(n)} \subset \mathcal{V}_{her}$ be the magic cone. We define the minimal magic operator system $\mathcal{S}^{(n)} = \bigcup\limits_{s \in \mathbb{N}} \mathcal{S}^{(n)}_s$ with

$$\mathcal{S}^{(n)}_s := \left\{ \sum_{\pi \in S_n} P_\pi \otimes q_\pi \mid P_\pi \in \mathrm{Mat}_n(\mathbb{C}) \text{ is permutation matrix},\ q_\pi \in \mathrm{PSD}_s \right\}$$

Remark 2.32. Note that, since the permutation matrices are the extreme rays of $\mathcal{C}^{(n)}$ (Lemma 2.29), we have

$$\begin{aligned} \mathcal{S}^{(n)}_s &:= \left\{ \sum_{\pi \in S_n} P_\pi \otimes q_\pi \mid P_\pi \in \mathrm{Mat}_n(\mathbb{C}) \text{ is permutation matrix},\ q_\pi \in \mathrm{PSD}_s \right\} \\ &= \left\{ \sum_{i=1}^{k} c_i \otimes q_i \mid k \in \mathbb{N},\ c_i \in \mathcal{C}^{(n)},\ q_i \in \mathrm{PSD}_s \right\} \end{aligned}$$

So it is indeed the minimal operator system containing $\mathcal{C}^{(n)}$ as described in for example [10].

Lemma 2.33. The minimal magic operator system is minimal in the sense that for all operator systems $\bigcup\limits_{s \in \mathbb{N}} D_s$ with $D_1 = \mathcal{C}^{(n)}$ it follows that $\forall s \in \mathbb{N} :\ \mathcal{S}^{(n)}_s \subseteq D_s$.

The proof of this lemma can be found in the appendix, Lemma 9.10. To prove it, we will use $\mathcal{V}^{(n)} \cong \mathbb{C}^m$ for some m and we consider the minimal operator system for any closed salient convex cone $C \subseteq \mathbb{R}^m$

Definition 2.34 (Maximal Magic Operator System)**.** Let $\mathcal{C}^{(n)} \subset \mathcal{V}_{her}$ be the magic cone. Then the maximal magic operator system is given by:

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

We write

$$\mathcal{L}^{(n)} = \bigcup_{s \in \mathbb{N}} \mathcal{L}_s^{(n)}$$

Lemma 2.35. $\mathcal{L}^{(n)}$ is maximal in the sense that for any operator system $\bigcup_{s \in \mathbb{N}} D_s$ with $D_1 \subseteq \mathcal{C}^{(n)}$ it holds that $D_s \subseteq \mathcal{L}_s^{(n)}$.

Again, the proof can be found in the appendix, Lemma 9.12.

Remark 2.36. (1) These operator systems are connected to the quantum magic squares in the following way:

$$\mathcal{M}_s^{(n)} = \{A \in \mathcal{L}_s^{(n)} \mid \forall i, j : \sum_k A_{i,k} = \sum_k A_{k,j} = \mathrm{I}_s\}$$

and

$$\mathcal{SC}_s^{(n)} = \{A \in \mathcal{S}_s^{(n)} \mid \forall i, j : \sum_k A_{i,k} = \sum_k A_{k,j} = \mathrm{I}_s\}.$$

(2) For $n \leq 2$ we have $\mathcal{S}^{(n)} = \mathcal{L}^{(n)}$.
For all $n \geq 3$ and $s \geq 2$ we have

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

since from Lemma 5 we know that $\mathcal{C}^{(n)}$ is not a simplex cone for $n \geq 3$. In [10], Theorem 4.7, it is shown that the minimal and maximal operator system over a convex cone C coincide if and only if the cone is a simplex.

2.4 Characterization of Semiclassical Quantum Magic Squares

In this section, we will take a closer look at semiclassical quantum magic squares. We will see that $\mathcal{SC}^{(n)} = mconv(\mathcal{CP}^{(n)})$ and give some further characterizations, using the notion of positive unital $*$-linear maps. The name describes the notion quite well, a definition can be found in the Appendix 9.2.
We will also show that for $n \geq 3, s \geq 2$ there exist quantum magic squares that are not semiclassical.
The whole section will follow the results of [8], Section 3.1.

Theorem 2.37. For any $n \in \mathbb{N}$ we have:

(1) $\mathcal{SC}^{(n)} = mconv(\mathcal{CP}^{(n)})$

(2) Let $A = (A_{i,j})_{i,j} \in \mathcal{M}_s^{(n)}$ be a quantum magic square. Consider the C^*-algebra $\mathbb{C}^{S_n} := \{f : \ S_n \to \mathbb{C}\}$ and let $f_{i,j} \in \mathbb{C}^{S_n}$ be defined as

$$\begin{aligned} f_{i,j} :\ S_n &\to \mathbb{C} \\ \pi &\mapsto \begin{cases} 1 & : \pi(i) = j \\ 0 & : \text{else} \end{cases} \end{aligned}$$

Then A is semiclassical if and only if there exists a positive unital $*$-linear map $\varphi : \mathbb{C}^{S_n} \to \mathrm{Mat}_s(\mathbb{C})$ such that $\varphi(f_{i,j}) = A_{i,j}$

(3) If $A = (A_{i,j})_{i,j} \in \mathcal{M}_s^{(n)}$ and for all $\pi \in S_n$ we have

$$\sum_{k=1}^{n} A_{k,\pi(k)} \geq \frac{n-2}{n-1} \cdot \mathrm{I}_s$$

then $A \in \mathcal{SC}_s^{(n)}$.

Proof. (1): In Proposition 2.25 we have seen that $\mathcal{SC}^{(n)} = mconv(\mathcal{P}_1^{(n)})$ so it suffices to show $\mathcal{P}_1^{(n)} \subseteq \mathcal{CP}^{(n)} \subseteq \mathcal{SC}^{(n)}$.
The first inclusion trivially holds, since the multiplication in $\mathbb{R}$ is commutative.

To see the other inclusion $\mathcal{CP}^{(n)} \subseteq \mathcal{SC}^{(n)}$, let $U = (u_{i,j})_{i,j} \in \mathcal{CP}_t^{(n)}$.
For any permutation $\pi \in S_n$ set

$$q_\pi := \prod_{k=1}^{n} u_{k,\pi(k)}.$$

Note that the $u_{i,j}$'s commute, thus the order of the product is not relevant.
Let P_π denote, as usual, the permutation matrix corresponding to π. And we will use $f_{i,j}$ as in Theorem 2.37 (2).

$$\begin{aligned} \left(\sum_{\pi \in S_n} P_\pi \otimes q_\pi \right)_{i,j} &= \sum_{\pi \in S_n} (P_\pi \otimes q_\pi)_{i,j} = \sum_{\pi \in S_n} f_{i,j}(\pi) \left(\prod_{k=1}^{n} u_{k,\pi(k)} \right) \\ &= u_{i,j} \underbrace{\left(\sum_{\pi \in S_n} f_{i,j}(\pi) \prod_{k \neq i} u_{k,\pi(k)} \right)}_{=:(*)} \end{aligned}$$

If we can show that $(*) = \mathrm{I}_t$, then we have shown that

$$U = \sum_{\pi \in S_n} P_\pi \otimes q_\pi \Rightarrow U \in \mathcal{SC}^{(n)}$$

For easier notation, we will only look at the case where $i = j = n$, but the other cases can be solved similarly.
Since $\mathcal{CP}^{(n)} \subseteq \mathcal{P}^{(n)}$, Proposition 2.16 states that

$$u_{i,k} u_{j,k} = 0$$

for all $i, j, k \in \{1, \ldots, n\}, i \neq j$.
Hence given a function $g : \{1, \ldots, n\} \to \{1, \ldots, n\}$ we have

$$\prod_{k=1}^{n} u_{k,g(k)} \neq 0 \iff g \text{ surjective } \iff g \in S_n.$$

Therefore we get

$$(*) = \sum_{\pi \in S_n} f_{n,n}(\pi) \prod_{k=1}^{n-1} u_{k,\pi(k)} = \sum_{\substack{g:\{1,\ldots,n\}\to\{1,\ldots,n\} \\ g(n)=n}} \prod_{k=1}^{n-1} u_{k,g(k)}$$

$$= \sum_{g:\{1,\ldots,n-1\}\to\{1,\ldots,n\}} \prod_{k=1}^{n-1} u_{k,g(k)} = \sum_{\ell=1}^{n-1} \sum_{\tau_\ell=1}^{n} \prod_{k=1}^{n-1} u_{k,\tau_k} \overset{(I)}{=} \prod_{k=1}^{n-1} \sum_{\tau=1}^{n} u_{k,\tau} \overset{(II)}{=} \mathrm{I}_t\,.$$

Seeing that equality (I) holds is probably easiest when looking at it from right to left, then it is just expansion of the product.
(II) follows from the fact that $(u_{i,j})_{i,j}$ is a quantum magic square.

The proof of part (2) and (3) are a bit off the topic of this work, so they will be skipped here but can be found in [8]. □

Remark 2.38. The quantum magic square filled with normalized identity matrices $\left(\frac{1}{n}\,\mathrm{I}_s\right)_{i,j=1}^{n} \in \mathcal{M}_s^{(n)}$ fulfils condition (3) of Theorem 2.37. This constant quantum magic square is a relative interior point of $\mathcal{M}_s^{(n)}$, hence condition (3) can be seen as a lower bound on the diameter of $\mathcal{SC}^{(n)}$ inside $\mathcal{M}^{(n)}$.

Before we can prove the final statement in this section, we need a preparatory lemma.

Lemma 2.39. Let $t > s \in \mathbb{N}$, $U \in \mathrm{Mat}_s(\mathbb{C})$ be a projector and let $W \in \mathrm{Mat}_t(\mathbb{C})$ such that $W \geq 0$, $\mathrm{I}_t - W \geq 0$ (i.e. W is a positive semi-definite contraction) and there exists an isometry $V \in \mathrm{Mat}_{t,s}(\mathbb{C})$ such that

$$U = V^* W V.$$

Then there exists some contraction $P \in \mathrm{Mat}_{t-s}(\mathbb{C})$, $P \geq 0, \mathrm{I}_{t-s} - P \geq 0$, such that, up to changing basis,

$$W = \begin{pmatrix} U & 0 \\ 0 & P \end{pmatrix}$$

i.e. W is the direct sum of U and P with respect to the decomposition $\mathbb{C}^t = V\mathbb{C}^s \oplus (V\mathbb{C}^s)^\perp$.

Proof. Write W with respect to the above decomposition:

$$W = \begin{pmatrix} U & R \\ R^* & P \end{pmatrix}$$

for some matrices $R \in \mathrm{Mat}_{s,t-s}(\mathbb{C}), P \in \mathrm{Mat}_{t-s}(\mathbb{C})$.
Since W is a contraction, we get

$$\begin{pmatrix} U & R \\ R^* & P \end{pmatrix} = W \geq W^2 = \begin{pmatrix} U^2 + RR^* & UR + RP \\ R^*U + PR^* & R^*R + P^2 \end{pmatrix} = \begin{pmatrix} U + RR^* & UR + RP \\ R^*U + PR^* & R^*R + P^2 \end{pmatrix}$$

Note that for matrices A, B we denote $A \geq B \iff A - B \geq 0$.
Hence the above calculation yields

$$\begin{pmatrix} -RR^* & R - UR - RP \\ R^* - R^*U - PR^* & P - R^*R - P^2 \end{pmatrix} \geq 0.$$

A block matrix can only be positive semi-definite if each block on the diagonal is positive semi-definite. Hence we need $-RR^* \geq 0$ but $RR^* \geq 0$ since it is a conjugate square. Therefore, $RR^* = 0$ which implies that $R = 0$ (since $(RR^*)_{i,i} = \sum_k R_{i,k}\overline{R_{i,k}} = \sum_k |R_{i,k}|^2$ is a sum of non-negative elements for every i).
But then also $P \geq P^2$ has to hold and we get the desired direct sum decomposition. $\square$

Finally, we can now show that there are quantum magic squares and for exterior size $n \geq 4$ even quantum permutation matrices that are not semiclassical.

Corollary 2.40. (1) For every $n \geq 3, s \geq 2$ we have

$$\mathcal{SC}_s^{(n)} \subsetneq \mathcal{M}_s^{(n)}$$

and in particular

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

(2) For $n \leq 3$ we have $\mathcal{SC}^{(n)} \supseteq \mathcal{P}^{(n)}$
For every $n \geq 4$ and $s \geq 2$ there exists a quantum permutation matrix which is not semiclassical, i.e. $\mathcal{SC}_s^{(n)} \supsetneq \mathcal{P}_s^{(n)}$.

Proof. (1) Let $n \geq 3, s \geq 2$. From Remark 2.36 (2) we know that

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

i.e. the maximal magic operator system at level s is strictly larger than the minimal magic operator system.
Therefore, we can find an $A \in \mathcal{L}_s^{(n)} \setminus \mathcal{S}_s^{(n)}$. The condition for being in $\mathcal{L}_s^{(n)}$ implies that for all $i, j \in \{1, \ldots, n\}$ and for all $v \in \mathbb{C}^s : v^*A_{i,j}v \geq 0$, in other words each entry of A is positive semi-definite. Therefore, the row and column sum matrix $a = \sum_k A_{i,k} = \sum_k A_{k,j}$ is positive semi-definite as well. But we need that a is positive definite, i.e. 0 is not an eigenvalue.
We know that $\mathcal{S}_s^{(n)}, \mathcal{L}_s^{(n)}$ are closed convex cones with non-empty interior. Hence also $\mathcal{L}_s^{(n)} \setminus \mathcal{S}_s^{(n)}$ has non-empty interior and we can therefore alter A a little bit, such that the row/column sum is positive definite but we are still in $\mathcal{L}_s^{(n)} \setminus \mathcal{S}_s^{(n)}$.

Hence, we can assume that the row/column sum a is positive definite.
Then we can find an invertible matrix $W \in \mathrm{Mat}_s(\mathbb{C})$ such that $W^*aW = \mathrm{I}_s$. Therefore, we get a quantum magic square $W^*AW = (W^*A_{i,j}W)_{i,j}$ that is not semiclassical, hence not in $\mathcal{S}_s^{(n)}$. If it would be semiclassical, we could find a representation $W^*AW = \sum_\pi P_\pi \otimes q_\pi$ and then $A = \sum_\pi P_\pi \otimes (W^{-1})^* q_\pi W^{-1} \in \mathcal{S}_s^{(n)}$, a contradiction.

(2) For $n \leq 3$ we have $\mathcal{CP}^{(n)} = \mathcal{P}^{(n)}$ which directly implies the first statement.
For $n \geq 4, s \geq 2$ there exists $U \in \mathcal{P}_s^{(n)} \setminus \mathcal{CP}_s^{(n)}$ (see Remark 2.18). If U was semiclassical, then by Theorem 2.37 we have $U \in mconv(\mathcal{CP}^{(n)})$, i.e. there exists $W \in \mathcal{CP}^{(n)}$ and an isometry V such that $U_{i,j} = V^*W_{i,j}V$. By Lemma 2.39 we can assume that there is a contraction $P_{i,j}$ such that

$$W_{i,j} = \begin{pmatrix} U_{i,j} & 0 \\ 0 & P_{i,j} \end{pmatrix}$$

But this gives a contradiction, since we assumed that the $U_{i,j}$ do not all commute. □

2.5 Matrix Convex Hull of Permutation Matrices/ Generalization of Birkhoff-von Neumman's Theorem

In this section, we will formulate a generalization of Birkhoff-von Neumann's Theorem to the setting of quantum magic squares. Instead of taking the convex hull, we will take the matrix convex hull and not just of the permutation matrices but the quantum permutation matrices. In contrast to the classical case, we will see that this matrix convex hull does not give the full set of quantum magic squares.
Again, we will follow [8] closely.

Theorem 2.41. For every $n \geq 3$ we have

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

The difference already appears at level $s = 2$.

From Remark 2.18 we know that for $n = 3$ we have $\mathcal{CP}^{(3)} = \mathcal{P}^{(3)}$. Therefore, Corollary 2.40 already gives the desired result, namely $mconv(\mathcal{P}^{(3)}) = mconv(\mathcal{CP}^{(3)}) \subsetneq \mathcal{M}^{(3)}$.
For $n \geq 4$ we will need some more work and proceed as follows: First, we will establish a necessary condition for being in the matrix convex hull of $\mathcal{P}^{(n)}$ (Proposition 2.43), then we will show that there is a quantum magic square in $\mathcal{M}_2^{(3)}$ which does not fulfil this condition. In the last step, we will embed it into quantum magic squares of larger size n and show that the necessary condition still fails.

Construction 2.42. Let $A = (A_{i,j})_{i,j} \in \mathcal{M}_s^{(n)}$. Then $\operatorname{col}(A)$ denotes the matrix we get by writing the entries of A in one column vector, the pairs of indices are ordered lexicographically, i.e. we get

$$\operatorname{col}(A) = \begin{pmatrix} A_{1,1} \\ A_{1,2} \\ \vdots \\ A_{2,1} \\ \vdots \\ A_{n,n} \end{pmatrix}.$$

Let $\{e_i\}_{i=1}^n$ denote the standard basis of $\mathbb{C}^n$. Then we can see $\operatorname{col}(A)$ as an element of a threefold tensor product as follows:

$$\operatorname{col}(A) = \sum_{i,j=1}^{n} e_i \otimes e_j \otimes A_{i,j} \in \mathbb{C}^n \otimes \mathbb{C}^n \otimes \operatorname{Her}_s(\mathbb{C})$$

$\operatorname{diag}(A)$ is defined similarly, we write the entries of A in the diagonal:

$$\operatorname{diag}(A) := \sum_{i,j=1}^{n} E_{i,i} \otimes E_{j,j} \otimes A_{i,j} \in \operatorname{Mat}_n(\mathbb{C}) \otimes \operatorname{Mat}_n(\mathbb{C}) \otimes \operatorname{Her}_s(\mathbb{C})$$

where $\{E_{i,j}\}_{i,j=1}^n$ is the canonical basis of $\operatorname{Mat}_n(\mathbb{C})$.
Furthermore, we will set

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

For $n = 2$ this matrix looks as follows:

$$\varphi(A) = \begin{pmatrix} A_{11} - A_{11}^2 & -A_{11}A_{12} & -A_{11}A_{21} & -A_{11}A_{22} \\ -A_{12}A_{11} & A_{12} - A_{12}^2 & -A_{12}A_{21} & -A_{12}A_{22} \\ -A_{21}A_{11} & -A_{21}A_{12} & A_{21} - A_{21}^2 & -A_{21}A_{22} \\ -A_{22}A_{11} & -A_{22}A_{12} & -A_{22}A_{21} & A_{22} - A_{22}^2 \end{pmatrix}$$

Additionally, we define for $n \geq 3$

$$\psi(A) := \sum_{\substack{i,j,k,l=1 \\ i \neq j, k \neq l}}^{n} E_{i,j} \otimes E_{k,l} \otimes (-\alpha_n \operatorname{I}_s + \beta_n A_{i,k} + \beta_n A_{j,l} + \gamma_n A_{i,l} + \gamma_n A_{j,k})$$

where

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

Lastly, let $\mathcal{Z}^{(n)} := \{M \in \operatorname{Mat}_n(\mathbb{C}) \mid \forall i \in \{1, \ldots, n\} : M_{i,i} = 0\}$ denote the vector space of matrices with zero on the diagonal and for $e := (1, \ldots, 1)^T \in \mathbb{C}^n$ we define

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

With this construction we can now formulate the desired necessary condition for being in $mconv(\mathcal{P}^{(n)})$.

Proposition 2.43. If $A \in mconv(\mathcal{P}^{(n)})_s$ then the following two formulas hold:

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

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

Furthermore, for any $A \in \mathcal{M}_s^{(n)}$ the formulas (1) and (2) are equivalent.

We will not prove this very technical proposition here. The proof can be found in [8].

Proof of Theorem 2.41. We will show the following statement by induction on n:
For all $n \geq 3$ there exists an element in $\mathcal{M}_2^{(n)}$ that does not satisfy (1) from Proposition 2.43.
For $n = 3$, we have already seen that $mconv(\mathcal{P}^{(3)})_2 \subsetneq \mathcal{M}_2^{(3)}$. Hence there are elements in $\mathcal{M}_2^{(n)} \setminus mconv(\mathcal{P}^{(n)})_2$ which makes it plausible that one of them does not satisfy (1). But we only know that (1) is a necessary condition, so we still need to prove the statement for $n = 3$. [8] provides us with an explicit example: 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 choose $A_{1,3}, A_{2,3}, A_{3,1}, A_{3,2}, A_{3,3}$ such that $A = (A_{i,j})_{i,j=1}^3 \in \mathcal{M}_2^{(3)}$.
Then A does not satisfy (2) from Proposition 2.43, hence it also does not satisfy (1) and is not in $mconv(\mathcal{P}^{(3)})$. This has been shown in [8] with the help of a computer algebra system. We will not go into further details here but instead move on to the induction step.
Let $n > 3$. By the induction hypothesis there exists an element $A \in \mathcal{M}_2^{(n-1)}$ which does not satisfy (1).
Now consider

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

We claim that $\tilde{A}$ does not satisfy (1) either.
Let $\tilde{X} \in (\mathcal{Z}^{(n)} \otimes \mathcal{Z}^{(n)} \otimes \mathrm{Mat}_2(\mathbb{C}))_{her}$ be arbitrary and let

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

Then

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

and

$$\begin{aligned}
&(v \otimes v \otimes \mathrm{I}_2)^* \varphi(\tilde{A})(v \otimes v \otimes \mathrm{I}_2) \\
&= (v^* \otimes v^* \otimes \mathrm{I}_2)\left(\sum_{i,j=1}^{n} E_{i,i} \otimes E_{j,j} \otimes \tilde{A}_{i,j} - \sum_{i,j,k,\ell=1}^{n} e_i e_k^* \otimes e_j e_\ell^* \otimes \tilde{A}_{i,j}\tilde{A}_{k,\ell}\right)(v \otimes v \otimes \mathrm{I}_2) \\
&= \sum_{i,j=1}^{n} v^* E_{i,i} v \otimes v^* E_{j,j} v \otimes \tilde{A}_{i,j} - \sum_{i,j,k,\ell=1}^{n} v^* E_{i,k} v \otimes v^* E_{j,\ell} v \otimes \tilde{A}_{i,j}\tilde{A}_{k,\ell} \\
&= \sum_{i,j=1}^{n-1} E_{i,i}^{(n-1)} \otimes E_{j,j}^{(n-1)} \otimes \tilde{A}_{i,j} - \sum_{i,j,k,\ell=1}^{n-1} E_{i,k}^{(n-1)} \otimes E_{j,\ell}^{(n-1)} \otimes \tilde{A}_{i,j}\tilde{A}_{k,\ell} = \varphi(A).
\end{aligned}$$

Where $E_{i,j}$ and $E_{i,j}^{(n-1)}$ are the canonical basis of $\mathrm{Mat}_n(\mathbb{C})$ and $\mathrm{Mat}_{n-1}(\mathbb{C})$, respectively. We used that for $1 \leq i, j \leq n-1$ we have $\tilde{A}_{i,j} = A_{i,j}$.
Therefore our induction hypothesis gives

$$(v \otimes v \otimes \mathrm{I}_2)^*(\varphi(\tilde{A}) + \tilde{X})(v \otimes v \otimes \mathrm{I}_2) = \varphi(A) + X \not\succeq 0$$

Thus it directly follows that

$$\varphi(\tilde{A}) + \tilde{X} \not\succeq 0$$

Since $\tilde{X}$ was chosen arbitrarily, the claim follows. $\square$

3 Quantum Latin Squares

In this section, we will have a look at another classical structure - Latin squares - and their quantum generalization as it was introduced by Benjamin Musto and Jamie Vicary in [19].

Definition 3.1. $L \in \mathrm{Mat}_n(\{1, \ldots, n\})$ is called a Latin square of size n if each number from $\{1, \ldots, n\}$ appears exactly once in each row and each column of L.

Latin squares are know by mathematicians for more than 300 years now. The Korean mathematician Choi Seok-Jeong used Latin squares in 1700 AD to construct magic squares [7]. Leonhard Euler (1707-1783) worked with Latin squares as well. He used Latin characters as symbols in his squares which is why they are now called "Latin squares".
A very popular application of a special case of Latin squares are the Sudoku puzzles. Here the player has to fill in the missing numbers of a 9×9 Latin

square with some extra condition on smaller 3×3 subsquares.
But Latin squares also have several applications in mathematics, for example in the design of experiments [1] and as multiplication tables of quasigroups [27].

The idea of Musto and Vicary was now to use quantum states as entries of an $n \times n$ square instead of numbers. From a mathematicians perspective, a quantum state basically is a normalized vector in some $\mathbb{C}^n$.
They translate the condition of "each number appearing exactly once" into "each direction of $\mathbb{C}^n$ appearing exactly once". This led to the following definition.

Definition 3.2. $L \in \mathrm{Mat}_n(\mathbb{C}^n)$ is called a quantum Latin square of size n if each row and each column of L forms an orthonormal basis of $\mathbb{C}^n$.

Example 3.3. (1) The easiest way to construct a quantum Latin square is to take a Latin square and an orthonormal basis of the correct size and arrange the basis according to the Latin square.
For example given the 4×4 Latin square

1	2	3	4
2	4	1	3
3	1	4	2
4	3	2	1

and some orthonormal basis $v_1, \ldots, v_4 \in \mathbb{C}^4$ we get the following quantum Latin square:

v_1	v_2	v_3	v_4
v_2	v_4	v_1	v_3
v_3	v_1	v_4	v_2
v_4	v_3	v_2	v_1

(2) But there are more quantum Latin squares than the ones we get with the above construction as this example of a quantum Latin square from [19] shows.

v_1	v_2	v_3	v_4
$\frac{1}{\sqrt{2}}(v_2 - v_3)$	$\frac{1}{\sqrt{5}}(iv_1 + 2v_4)$	$\frac{1}{\sqrt{5}}(2v_1 + iv_4)$	$\frac{1}{\sqrt{2}}(v_2 + v_3)$
$\frac{1}{\sqrt{2}}(v_2 + v_3)$	$\frac{1}{\sqrt{5}}(2v_1 + iv_4)$	$\frac{1}{\sqrt{5}}(iv_1 + 2v_4)$	$\frac{1}{\sqrt{2}}(v_2 - v_3)$
v_4	v_3	v_2	v_1

Here $v_1, \ldots, v_4 \in \mathbb{C}^n$ is again some arbitrary fixed orthonormal basis. But in this square a total of four different orthonormal bases can be found in the rows and columns.

3.1 Hadamard Matrices and Unitary Error Bases

Next, we will define unitary error bases, also known as unitary operator bases. These structures are used in quantum information theory, for example in quantum teleportation, dense coding and error correction [19]. Unitary error bases

are hard to find [17]. We will take a look at the quantum shift-and-multiply method introduced in [19] that uses a family of Hadamard matrices and a quantum Latin square to construct a unitary error basis.
We start with the definitions, following [19].

Definition 3.4. A Hadamard matrix of size n is an $n \times n$ complex matrix H satisfying the following conditions for all $i, j \in \{1, \dots, n\}$:

(1) $|H_{i,j}| = 1$

(2) $HH^* = n\,\mathrm{I}_n$

(3) $H^*H = n\,\mathrm{I}_n$

Example 3.5. An example of a Hadamard matrix of size 4 is

$$H = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}.$$

Definition 3.6. A set $\mathcal{E}$ of n^2 unitary $n \times n$ matrices is called unitary error basis if the elements in $\mathcal{E}$ are orthogonal with respect to the following inner product:

$$A, B \in \mathrm{Mat}_n(\mathbb{C}) : \langle A, B \rangle := \frac{1}{n} \operatorname{tr}(A^* B)$$

In particular, $\mathcal{E}$ forms an orthonormal basis of $\mathrm{Mat}_n(\mathbb{C})$ with respect to this inner product and the induced norm.

Example 3.7. The most well-known example of a unitary error basis that is widely used in quantum information theory are the Pauli matrices

$$\mathcal{P} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right\}$$

which form a unitary error basis of $\mathrm{Mat}_2(\mathbb{C})$.

Definition 3.8 (Quantum Shift-and-Multiply Method)**.** Given a quantum Latin square of size n Q and a family of $n \times n$ Hadamard matrices $\{H_j\}_{j=1}^n$. Then the associated quantum shift-and-multiply basis consists of the following elements, for $i, j \in \{1, \dots, n\}$:

$$S_{i,j} = Q_j \operatorname{diag}(H_j, i)$$

where

$$Q_j := (Q_{j,\ell})_{\ell=1}^n \in \mathrm{Mat}_n(\mathbb{C})$$

is the matrix whose columns are the entries of the $j-$th row of Q and $\operatorname{diag}(H_j, i)$ is the diagonal matrix whose diagonal entries are given by the $i-$th row of H_j, i.e. $\operatorname{diag}(H_j, i)_{\ell,k} = \delta_{\ell,k} \cdot (H_j)_{i,\ell}$.
In words: The $(i, j)-$th element of the quantum shift-and-multiply basis is the matrix given as the product of the $j-$th row of the quantum Latin square with diagonal matrix given by the $i-$th row of the $j-$th Hadamard matrix.

Remark 3.9. An explicit example of such a quantum shift-and-multiply basis constructed with the quantum Latin square from Example 3.3 (2) and Hadamard matrices $H_1 = \ldots = H_4 = H$ from Example 3.5 can be found in [19].

Next, we want to prove that our above construction gives indeed a unitary error basis.

Theorem 3.10. Quantum shift-and-multiply bases are unitary error bases.

To prove this theorem, we need two preparatory lemmas.

Lemma 3.11. An element $Q \in \mathrm{Mat}_n(\mathbb{C}^n)$ is a quantum Latin square if and only if it satisfies the following properties:

(1) For all $i \in \{1, \ldots, n\}$: Q_i is unitary, or equivalently $(Q_{i,k})^*(Q_{i,\ell}) = \delta_{k,\ell}$ for all $k, \ell \in \{1, \ldots, n\}$.

(2) For all $i, k, \ell \in \{1, \ldots, n\}$: $(Q_{k,i})^* Q_{\ell,i} = \delta_{k,\ell}$.

Note that $Q_{i,j} \in \mathbb{C}^n$.

Proof. Q_i is unitary per definition if $Q_i^* Q_i = \mathrm{I}_n$. Hence

$$\delta_{k,\ell} = (Q_i^* Q_i)_{k,\ell} = \sum_j (Q_i^*)_{k,j} (Q_i)_{j,\ell} = (Q_{i,k})^* Q_{i,\ell}.$$

Property (1) is equivalent to requiring that every row of Q forms an orthonormal basis, while property (2) is equivalent to saying that every column of Q forms an orthonormal basis, since we use the standard scalar product on $\mathbb{C}^n$: for $v, w \in \mathbb{C}^n : \langle v, w \rangle = v^* w$. □

Lemma 3.12. Let $D \in \mathrm{Mat}_n(\mathbb{C})$ be a diagonal matrix and $A \in \mathrm{Mat}_n(\mathbb{C})$ be zero on the main diagonal. Then $(DA)_{i,i} = 0$ for all $i \in \{1, \ldots, n\}$.

Proof. Let $i \in \{1, \ldots, n\}$ arbitrary. We look at the i-th entry of the product on the diagonal:

$$(DA)_{i,i} = \sum_j D_{i,j} A_{j,i} = \sum_j \delta_{i,j} D_{i,i} A_{j,i} = D_{i,i} A_{i,i} = 0.$$

□

Now we can tackle the proof of Theorem 3.10, following the argument in [19].
Proof of Theorem 3.10.
So let Q be a quantum Latin square of size n and $H_1, \ldots, H_n \in \mathrm{Mat}_n(\mathbb{C})$ be a family of Hadamard matrices.
Before we start with the arguments for the proof, we quickly revise the notation:

- $Q_i \in \mathrm{Mat}_n(\mathbb{C})$ the i-th row of Q put together into one matrix.
- $Q_{i,j} \in \mathbb{C}^n$ the column vector at position i, j in Q.

- $Q_{i,j,k} = (Q_{i,j})_k$ the k-th entry of the column at position i, j.

Note that $(Q_i)_{k,\ell} = Q_{i,\ell,k}$ since we look at the i-th row of Q, the ℓ-th column and then the k-th entry in this vector.

Set $S_{i,j} = Q_j \operatorname{diag}(H_j, i)$.
First, observe that Q_j is unitary by Lemma 3.11 and $\operatorname{diag}(H_j, i)$ is unitary since it is a diagonal matrix with unit complex numbers on the diagonal. Hence, $S_{i,j}$ is unitary as the product of two unitary matrices.
Next, we need to show the orthogonality, namely that

$$\frac{1}{n}\operatorname{tr}(S_{i,j}^* S_{k,\ell}) = \delta_{i,k}\delta_{j,\ell}$$

holds.
If $i = k, j = \ell$, the unitarity of $S_{i,j}$ implies

$$\frac{1}{n}\operatorname{tr}(S_{i,j}^* S_{i,j}) = \frac{1}{n}\operatorname{tr}(\mathrm{I}_n) = 1.$$

If $j = \ell$ but $i \neq k$ we get

$$\begin{aligned}\operatorname{tr}(S_{i,j}^* S_{k,j}) &= \operatorname{tr}(\operatorname{diag}(H_j, i)^* Q_j^* Q_j \operatorname{diag}(H_j, k))\\ &= \operatorname{tr}(\operatorname{diag}(H_j, i)^* \operatorname{diag}(H_j, k)) = \sum_{\ell} \overline{(H_j)_{i,l}}(H_j)_{k,l} = (H_j H_j^*)_{k,i} = 0.\end{aligned}$$

In the last step, we used that distinct rows of a Hadamard matrix are orthogonal to each other, which is given by condition (2) in Definition 3.4.
Lastly, we consider the case $j \neq \ell$.
We use the cyclic property of the trace to obtain

$$\begin{aligned}\operatorname{tr}(S_{i,j}^* S_{k,\ell}) &= \operatorname{tr}(\operatorname{diag}(H_j, i)^* Q_j^* Q_\ell \operatorname{diag}(H_\ell, k))\\ &= \operatorname{tr}(\operatorname{diag}(H_\ell, k)\operatorname{diag}(H_j, i)^* Q_j^* Q_\ell).\end{aligned}$$

The product $\operatorname{diag}(H_\ell, k)\operatorname{diag}(H_j, i)^*$ is again a diagonal matrix. On the other hand, for $p \in \{1, \ldots, n\}$ arbitrary, we have

$$(Q_j^* Q_\ell)_{p,p} = \sum_{q=1}^{n} (Q_j^*)_{p,q}(Q_\ell)_{q,p} \overset{(1)}{=} \sum_{q} \overline{Q_{j,p,q}} Q_{\ell,p,q} = (Q_{j,p})^* Q_{\ell,p} \overset{(2)}{=} 0$$

where we used the observation at the beginning of the proof for (1). In (2) we use the second part of Lemma 3.11.
Lemma 3.12 gives that

$$\operatorname{tr}(\operatorname{diag}(H_\ell, k)\operatorname{diag}(H_j, i)^* Q_j^* Q_\ell) = 0$$

as required. □

4 The Connection of Quantum Latin Squares and Quantum Magic Squares

In this section, we investigate how we can connect quantum Latin squares and quantum magic squares. This will give rise to several classes of quantum magic squares. We take a closer look at how these classes are related, also when taking the matrix convex hull. One result will be that the notion of semiclassical fits well to the setting of quantum Latin squares.

Proposition 4.1. Given a quantum Latin square $V = (v_{i,j})_{i,j=1}^n \in \mathrm{Mat}_n(\mathbb{C}^n)$ then

$$\left(v_{i,j}v_{i,j}^*\right)_{i,j=1}^n \in \mathrm{Mat}_n(\mathrm{Her}_n(\mathbb{C}))$$

is a quantum magic square.

Given a quantum magic square $A = (A_{i,j})_{i,j=1}^n \in \mathrm{Mat}_n(\mathrm{Her}_n(\mathbb{C}))$ with $\mathrm{rank}(A_{i,j}) = 1$ for all i, j then there exist $a_{i,j} \in \mathbb{C}^n$ such that $A_{i,j} = a_{i,j}a_{i,j}^*$ and

$$(a_{i,j})_{i,j=1}^n \in \mathrm{Mat}_n(\mathbb{C}^n)$$

is a quantum Latin square.

Proof. To show the first statement, let $V = (v_{i,j})_{i,j}$ be a quantum Latin square. Note that the rank one square vv^* is positive semi-definite for any $v \in \mathbb{C}^n$.
Fix some row $i \in \{1, \ldots, n\}$. Then $v_{i,1}, \ldots, v_{i,n} \in \mathbb{C}^n$ is an orthonormal basis, hence for any $k \in \{1, \ldots, n\}$ we get

$$\left(\sum_{j=1}^n v_{i,j}v_{i,j}^*\right) v_{i,k} = \sum_j v_{i,j} \underbrace{(v_{i,j}^* v_{i,k})}_{=\delta_{j,k}} = v_{i,k}.$$

In words, the sum $\sum_{j=1}^n v_{i,j}v_{i,j}^*$ acts like the identity on a basis of $\mathbb{C}^n$, hence $\sum_{j=1}^n v_{i,j}v_{i,j}^* = \mathrm{I}_n$.

The same argument also works for any column of V, therefore $\left(v_{i,j}v_{i,j}^*\right)_{i,j=1}^n \in \mathcal{M}_n^{(n)}$.

For the second statement, let $A = (A_{i,j})_{i,j} \in \mathcal{M}_n^{(n)}$ such that for all i, j we have $\mathrm{rank}(A_{i,j}) = 1$. Since A is a quantum magic square, we have $A_{i,j} \geq 0$. Hence each entry of A can be written as a conjugate square of a matrix of size $n \times \mathrm{rank}(A_{i,j})$, i.e. there exist some $a_{i,j} \in \mathbb{C}^n$ such that $A_{i,j} = a_{i,j}a_{i,j}^*$.
We now have to show that, for all i, j, $a_{i,1}, \ldots, a_{i,n}$ and $a_{1,j}, \ldots, a_{n,j}$ form orthonormal bases of $\mathbb{C}^n$.
Fix some row $i \in \{1, \ldots, n\}$.
Assume for the sake of contradiction that $a_{i,1}, \ldots, a_{i,n}$ are not linearly independent, i.e. there exist $\lambda_j \in \mathbb{C}$ such that

$$a_{i,1} = \sum_{j=2}^n \lambda_j a_{i,j}.$$

Thus

$$a_{i,1}a_{i,1}^* = \left(\sum_{j=2}^{n} \lambda_j a_{i,j}\right)\left(\sum_{k=2}^{n} \lambda_k a_{i,k}\right)^* = \sum_{k=2}^{n} \overline{\lambda_k}\left(\underbrace{\sum_{j=2}^{n} \lambda_j a_{i,j}}_{=:v_i}\right) a_{i,k}^*.$$

Then, since A is a quantum magic square, we get

$$\mathrm{I}_n = \sum_{j=1}^{n} a_{i,j}a_{i,j}^* = \sum_{k=2}^{n} \overline{\lambda_k} v_i a_{i,k}^* + \sum_{j=2}^{n} a_{i,j}a_{i,j}^* = \sum_{j=2}^{n}\left(\underbrace{\overline{\lambda_k} v_i + a_{i,j}}_{=:w_{i,j}}\right) a_{i,j}^*.$$

But on the other hand

$$n = \operatorname{rank}(\mathrm{I}_n) = \operatorname{rank}\left(\sum_{j=2}^{n} w_{i,j}a_{i,j}^*\right) \leq \sum_{j=2}^{n} \operatorname{rank}(w_{i,j}a_{i,j}^*) = n-1$$

which gives the desired contradiction.
Hence $a_{i,1}, \ldots, a_{i,n}$ are linear independent and therefore a basis of $\mathbb{C}^n$.
To show the orthonormality we use the uniqueness of the representation of a vector with respect to a given basis.

$$a_{i,k} = \mathrm{I}_n\, a_{i,k} = \sum_{j=1}^{n} a_{i,j} \underbrace{a_{i,j}^* a_{i,k}}_{\in\mathbb{C}} \Rightarrow a_{i,j}^* a_{i,k} = \delta_{j,k}$$

In total, we have shown that any row of $(a_{i,j})_{i,j} \in \mathrm{Mat}_n(\mathbb{C}^n)$ gives rise to an orthonormal basis. An analogous argument shows the same for the columns of $(a_{i,j})_{i,j}$, hence it is a quantum Latin square. □

This proposition shows that quantum Latin squares can be understood as a special case of quantum magic squares. We will formalize this, and another way to construct quantum magic squares, in the next definition.

Definition 4.2. We will denote the set of quantum magic squares of exterior size n and interior size s, where each entry matrix has rank 1, with

$$\mathcal{RO}_s^{(n)} := \{A \in \mathcal{M}_s^{(n)} \mid \forall i,j \in \{1,\ldots,n\} : \operatorname{rank}(A_{i,j}) = 1\}$$

and set $\mathcal{RO}^{(n)} = \bigcup_{s\in\mathbb{N}} \mathcal{RO}_s^{(n)}$.
The set of embedded quantum Latin squares, that arise from a classical Latin square and one orthonormal basis as described in Example 3.3 (1), is denoted by

$$\mathcal{L}_n := \left\{ \left(v_{L_{i,j}} v_{L_{i,j}}^*\right)_{i,j=1}^{n} \mid L \text{ is classical Latin square of size } n, \right.$$
$$\left. v_1, \ldots, v_n \in \mathbb{C}^n \text{ orthonormal basis} \right\}.$$

Remark 4.3. (1) The set $\mathcal{RO}_n^{(n)}$ is in one to one correspondence with the set of quantum Latin squares of size n as shown in Proposition 4.1.
For $s > n$ the set $\mathcal{RO}_s^{(n)}$ is empty since less than s rank 1 matrices can not sum up to the identity matrix, since $\mathrm{rank}(\mathrm{I}_s) = s$.

(2) Every element from $\mathcal{RO}_n^{(n)}$ is a quantum permutation matrix, since each entry can be written as a conjugate square of a normalized vector as seen in Proposition 4.1. For a norm one vector $v \in \mathbb{C}^n$ we have $(vv^*)^2 = v(v^*v)v^* = vv^*$.
For $\mathcal{RO}_s^{(n)}$ with $s < n$ this is not the case, as the following example shows.

$$\begin{array}{|c|c|c|}\hline \frac{1}{2}e_1e_1^* & \frac{1}{2}e_1e_1^* & e_2e_2^* \\ \hline e_2e_2^* & \frac{1}{2}e_1e_1^* & \frac{1}{2}e_1e_1^* \\ \hline \frac{1}{2}e_1e_1^* & e_2e_2^* & \frac{1}{2}e_1e_1^* \\ \hline \end{array} \in \mathcal{RO}_2^{(3)}$$

Here $e_1, e_2 \in \mathbb{C}^2$ is the standard basis. But clearly this is not a quantum permutation matrix since $(\frac{1}{2}e_1e_1^*)^2 = \frac{1}{4}e_1e_1^*$.

(3) We have $\mathcal{L}_n \subseteq \mathcal{RO}_n^{(n)} \subseteq \mathcal{M}_n^{(n)}$, but we can also consider $\mathcal{L}_n \subseteq \mathcal{M}^{(n)}$. In that case all levels $s \neq n$ are empty.

(4) Furthermore, it holds that $\mathcal{L}_n \subseteq \mathcal{CP}_n^{(n)}$. Given some $\left(v_{L_{i,j}}v_{L_{i,j}}^*\right)_{i,j=1}^n \in \mathcal{L}_n$, each entry is per definition a rank one projector. These projectors commute, since

$$\begin{aligned} v_{L_{i,j}}v_{L_{i,j}}^* v_{L_{k,\ell}}v_{L_{k,\ell}}^* &= v_{L_{i,j}}\delta_{L_{i,j},L_{k,\ell}}v_{L_{k,\ell}}^* = \delta_{L_{i,j},L_{k,\ell}}v_{L_{i,j}}v_{L_{i,j}}^* \\ &= v_{L_{k,\ell}}v_{L_{k,\ell}}^* v_{L_{i,j}}v_{L_{i,j}}^*. \end{aligned}$$

The next proposition shows that we can consider $\mathcal{L}_n$ as the set of semiclassical quantum Latin squares. This makes sense, since the elements in $\mathcal{L}_n$ arise from classical Latin squares.

Proposition 4.4. For any $n \in \mathbb{N}$ we have

$$\mathcal{SC}^{(n)} \cap \mathcal{RO}_n^{(n)} = \mathcal{L}_n.$$

Proof. Let $A = \sum_{\pi \in S_n} P_\pi \otimes q_\pi$ be a semiclassical quantum magic square of size n such that each entry has rank 1. ($P_\pi \in \mathrm{Mat}_n(\mathbb{C})$ are permutation matrices, $q_\pi \in \mathrm{PSD}_n$, $\sum_\pi q_\pi = \mathrm{I}_n$.)
For two positive semi-definite matrices (of the same size) A, B, we have

$$\max\{\mathrm{rank}(A), \mathrm{rank}(B)\} \leq \mathrm{rank}(A+B) \leq \mathrm{rank}(A) + \mathrm{rank}(B).$$

Hence all the q_π have rank one and can therefore be written as a conjugate square of a vector.
For two rank one squares aa^*, bb^* $(a, b \in \mathbb{C}^n)$ it holds that

$$\mathrm{rank}(aa^* + bb^*) = 1 \iff \exists c \in \mathbb{C} : a = cb \vee b = 0.$$

Let $\Pi_{i,j} := \{\pi \in S_n | (P_\pi)_{i,j} = 1\}$.
For $\pi, \tilde{\pi} \in \Pi_{i,j}$ the above thoughts imply that:

$$\exists c \in \mathbb{C} : q_\pi = c q_{\tilde{\pi}} \vee q_{\tilde{\pi}} = 0.$$

In other words, $\dim_{\mathbb{C}}(\text{span}_{\mathbb{C}}\{q_\pi \mid \pi \in \Pi_{i,j}\}) = 1$ for all $i, j \in \{1, \ldots, n\}$ $(*)$.
Note that for all $i, j : A_{i,j} \neq 0$ because if one entry would be zero, w.l.o.g. assume $A_{1,1} = 0$, then

$$n = \text{rank}(\text{I}_n) = \text{rank}\left(\sum_{j=1}^{n} A_{1,j}\right) = \text{rank}\left(\sum_{j=2}^{n} A_{1,j}\right) \leq n - 1$$

a contradiction.
Fix for every $i \in \{1, ..., n\}$ a $\pi_i \in \Pi_{i,1}$ such that $q_{\pi_i} \neq 0$.
By a similar rank argument as above, we see that $A_{1,j} \notin \text{span}_{\mathbb{C}}(A_{1,\ell})$ for $j \neq \ell$. Hence $q_{\pi_j} \notin \text{span}_{\mathbb{C}}(q_{\pi_\ell})$ for $j \neq \ell$.
But on the other hand, $(*)$ holds, therefore if $\pi_l \in \Pi_{i,j}$ then for all $k \in \{1, \ldots, n\} \setminus \{l\} : \pi_k \notin \Pi_{i,j}$.
All in all, we have n permutations $\pi_1, \ldots, \pi_n$ that are completely disjoint in the sense that no two permutations map one input to the the same output. But then each possible mapping instruction $i \mapsto j$ has to be fulfilled by one of the π_k. Hence for all $i, j \in \{1, \ldots, n\}$ there exists a unique $\ell \in \{1, \ldots, n\}$ such that $\pi_\ell \in \Pi_{i,j}$.

Now let $\pi \in S_n \setminus \{\pi_1, ..., \pi_n\}$. We claim that $q_\pi = 0$.

We know that there exists some $\ell \in \{1, \ldots, n\}$ such that $\pi \in \Pi_{\ell,1}$. Since $\pi \neq \pi_\ell$ there exists some $j \in \{1, \ldots, n\} \setminus \{\ell\}$ such that $\pi(j) \neq \pi_\ell(j)$. Set $k = \pi(j)$, then $\pi \in \Pi_{j,k}$ and let i be such that $\pi_i \in \Pi_{j,k}$. Hence it has to hold that $q_\pi \in \text{span}_{\mathbb{C}}(q_{\pi_l}) \cap \text{span}_{\mathbb{C}}(q_{\pi_i}) = \{0\}$ which proves the claim.

All together, we have $A = \sum_{i=1}^{n} P_{\pi_i} \otimes q_{\pi_i}$. The q_{π_i} are rank 1 squares, i.e. $\exists Q_{\pi_i} \in \mathbb{C}^n : q_{\pi_i} = Q_{\pi_i} Q_{\pi_i}^*$. From Proposition 4.1 we can see that $Q_{\pi_1}, \ldots, Q_{\pi_n}$ form an orthonormal basis.
Earlier, we have seen that for each i, j there is one π_ℓ such that $\pi_\ell(i) = j$. Hence $\sum_{i=1}^{n} P_{\pi_i}$ gives the all one matrix and

$$\sum_{i=1}^{n} P_{\pi_i} \otimes i$$

is a Latin square, since each number appears exactly once in each row and each column.

To see that any element from $\mathcal{L}_n$ is semiclassical, note that we have shown $\mathcal{L}_n \subseteq \mathcal{CP}_n^{(n)}$ in Remark 4.3 (4). Together with Theorem 2.37, we get $\mathcal{L}_n \subseteq \mathcal{SC}_n^{(n)}$. $\square$

Definition 4.5. A special case of a positive operator valued measure (POVM, see Definition 2.10) is the so called projection valued measure (PVM) which are n positive semi-definite matrices $P_1, \dots, P_n \in \mathrm{Her}_s(\mathbb{C})$ such that each P_i is a projector ($P_i^2 = P_i$) and $\sum_{i=1}^n P_i = \mathrm{I}_n$.

Remark 4.6. Given a POVM or PVM and a Latin square, if we arrange the matrices according to the Latin square, similar to Example 3.3 (1), we get a quantum magic square. Because in this construction each matrix from the POVM/PVM appears exactly once in each row and each column, the matrices in each row and column will sum to the identity.

This remark motivates the following definition.

Definition 4.7. We define

$$\mathcal{POVMLS}_s^{(n)} := \left\{ \left(P_{L_{i,j}}\right)_{i,j=1}^n \mid P_1, \dots, P_n \in \mathrm{Her}_s(\mathbb{C}) \text{ is POVM, } L \text{ is Latin square of size } n \right\}$$
$$\mathcal{PVMLS}_s^{(n)} := \left\{ \left(P_{L_{i,j}}\right)_{i,j=1}^n \mid P_1, \dots, P_n \in \mathrm{Her}_s(\mathbb{C}) \text{ is PVM, } L \text{ is Latin square of size } n \right\}$$
$$\mathcal{POVMLS}^{(n)} := \bigcup_{s\in\mathbb{N}} \mathcal{POVMLS}_s^{(n)}, \quad \mathcal{PVMLS}^{(n)} := \bigcup_{s\in\mathbb{N}} \mathcal{PVMLS}_s^{(n)}.$$

Remark 4.8. Since each PVM is per definition also a POVM, we have

$$\mathcal{PVMLS}^{(n)} \subseteq \mathcal{POVMLS}^{(n)}.$$

In the next part, we will investigate some properties of the newly defined sets.

Lemma 4.9. Every element of $\mathcal{POVMLS}^{(n)}$ is semiclassical.

Proof. Let $A \in \mathcal{POVMLS}_s^{(n)}$ then there exists a POVM $A_1, ..., A_n \in \mathrm{Her}_s(\mathbb{C})$ and a Latin square of size n L that generate A. Analogues to the proof of 4.4, we define permutation matrices by setting for all $i, \ell, k \in \{1, \dots n\}$:

$$(P_i)_{\ell,k} = \begin{cases} 1 & \text{if } L_{\ell,k} = i \\ 0 & \text{else} \end{cases}$$

Then we can rewrite A as

$$A = \sum_{i=1}^n P_i \otimes A_i$$

Since the A_i form a POVM, they are positive semi-definite matrices summing to the identity. Hence A is semiclassical. $\square$

Lemma 4.10. The sets $\mathcal{RO}^{(n)}, \mathcal{L}_n, \mathcal{POVMLS}^{(n)}, \mathcal{PVMLS}^{(n)}$ are all closed with respect to simultaneous unitary conjugation, but not closed with respect to taking direct sums (for $n \geq 2$). Hence they are not free sets and in particular not matrix convex.

Proof. The matrix properties of having rank 1, being positive semi-definite or a projector are all preserved by unitary conjugation. Hence the first statement holds.
The direct sum of two rank one matrices cannot have rank one again. If A, B are rank one matrices, then they both have at least on nonzero row a, b respectively. In $A \oplus B$ there will be the rows $(a, 0, \ldots, 0)$ and $(0, \ldots, 0, b)$ which will clearly be linearly independent since there is no index where both are nonzero. But this directly implies $\operatorname{rank}(A \oplus B) \geq 2$.
Therefore $\mathcal{RO}^{(n)}$ and $\mathcal{L}_n$ cannot be closed under direct sums.
Taking direct sums of POVMs/PVMs will again give a POVM/PVM. But the problem is that the resulting quantum magic square might have different POVMs/PVMs in its rows or columns and thus it would not be generated by a Latin square any more.
Lastly, note that any matrix convex set has to be closed under direct sums.

□

Since these sets are not matrix convex, we will now investigate what we gain by taking the matrix convex hull.

Proposition 4.11. We have

$$mconv(\mathcal{PVMLS}^{(n)}) = mconv(\mathcal{POVMLS}^{(n)})$$

for any $n \in \mathbb{N}$.

Proof. From Remark 4.8 we know that $\mathcal{PVMLS}^{(n)} \subseteq \mathcal{POVMLS}^{(n)}$ and hence $mconv(\mathcal{PVMLS}^{(n)}) \subseteq mconv(\mathcal{POVMLS}^{(n)})$.
For the other direction, let $P \in \mathcal{POVMLS}_s^{(n)}$. Then there exists a POVM $B_1, ..., B_n \in \mathrm{Her}_s(\mathbb{C})$ and a Latin square L of size n, which give rise to P.
By Naimarks Dilation Theorem (see for example [23]) each POVM dilates to a PVM, i.e. there exist $m \in \mathbb{N}, V \in \mathrm{Mat}_{m,s}(\mathbb{C})$ with $V^*V = \mathrm{I}_s$ and a PVM $A_1, ..., A_n \in \mathrm{Her}_m(\mathbb{C})$ such that $B_i = V^*A_iV$ for all $i \in \{1, \ldots, n\}$.
Now let $C = \left(A_{L_{i,j}}\right)_{i,j=1}^n \in \mathcal{PVMLS}_m^{(n)}$ be the quantum magic square that we get by arranging $A_1, ..., A_n$ according to L. Then

$$\forall i, j \in \{1, \ldots, n\} : P_{i,j} = V^*C_{i,j}V \ .$$

Hence $P \in mconv(\mathcal{PVMLS}^{(n)})$. □

Theorem 4.12. For any $n \in \mathbb{N}$ we have that

$$mconv(\mathcal{PVMLS}^{(n)}) = mconv(\mathcal{L}_n).$$

Proof. First, note that give an orthonormal basis $v_1, \ldots, v_n \in \mathbb{C}^n$ the rank one squares $v_1v_1^*, \ldots, v_nv_n^*$ form a PVM since they are projectors and sum up to the identity as seen in Proposition 4.1 and Remark 4.3 (4). Hence $\mathcal{L}_n \subseteq \mathcal{PVMLS}^{(n)}$ and therefore $mconv(\mathcal{L}_n) \subseteq mconv(\mathcal{PVMLS}^{(n)})$.

For the other direction, let $P_1, ..., P_n \in \mathrm{Her}_s(\mathbb{C})$ be a PVM and L a Latin square of size n.
Since the P_i are orthogonal projections, each has a representation as a sum of rank one squares:

$$P_i = \sum_{\ell=1}^{r_i} p_\ell^{(i)} p_\ell^{(i)*}$$

where r_i is the rank of P_i and the $p_\ell^{(i)} \in \mathbb{C}^s$ are orthonormal.
Let $r = \max\{r_1, ..., r_n\}$ and set $p_\ell^{(i)} = 0$ for all $r_i < \ell \leq r$. Furthermore, we set

$$V_i^* := \left(p_i^{(1)} | \dots | p_i^{(n)}\right) \in \mathrm{Mat}_{s,n}(\mathbb{C})$$

and $a_i := e_i$ the standard basis of $\mathbb{C}^n$ for all $i \in \{1, \dots, n\}$.
Then

$$V_i^* a_j a_j^* V_i = p_i^{(j)} p_i^{(j)*}$$

and thus

$$\sum_{i=1}^{r} V_i^* a_j a_j^* V_i = \sum_{i=1}^{r_j} p_i^{(j)} p_i^{(j)*} = P_j.$$

Let $A = \left(a_{L_{i,j}} a_{L_{i,j}}^*\right)_{i,j} \in \mathcal{L}_n$ be the quantum magic square we get from the orthonormal basis $a_1, ..., a_n$ and the Latin square L.
If we can show that $\sum_i V_i^* V_i = \mathrm{I}_s$, then $\left(P_{L_{i,j}}\right)_{i,j} = \left(\sum_{i=1}^r V_i^* A_{i,j} V_i\right)_{i,j}$ is indeed a matrix convex combination of elements in $\mathcal{L}_n$.
For any $i \in \{1, \dots, n\}$ we have

$$V_i^* V_i = \left(p_i^{(1)} | \dots | p_i^{(n)}\right) \cdot \begin{pmatrix} p_i^{(1)*} \\ \vdots \\ p_i^{(n)*} \end{pmatrix} = \sum_{\ell=1}^{n} p_i^{(\ell)} p_i^{(\ell)*}$$

thus, and because the P_i form a PVM, we get:

$$\sum_{i=1}^{r} V_i^* V_i = \sum_{i=1}^{r} \sum_{l=1}^{n} p_i^{(l)} p_i^{(l)*} = \sum_{l=1}^{n} P_l = \mathrm{I}_s$$

$\square$

Theorem 4.13. For any $n \in \mathbb{N}$ we have that

$$mconv(\mathcal{CP}^{(n)}) = mconv(\mathcal{L}_n).$$

Proof. In Remark 4.3 (4) we showed that $\mathcal{L}_n \subseteq \mathcal{CP}^{(n)}$ hence also $mconv(\mathcal{L}_n) \subseteq mconv(\mathcal{CP}^{(n)})$.
For the other direction, we start by taking $P \in \mathcal{CP}_s^{(n)}$ such that all $P_{i,j}$ are

diagonal matrices and show that $P \in mconv(\mathcal{L}_n)$.
Fix arbitrary $i, j \in \{1, \dots, n\}$. Since $P_{i,j}$ is positive semi-definite and a diagonal matrix, all its entries have to be grater or equal to zero. Furthermore, $P_{i,j} = P_{i,j}^2 = \operatorname{diag}\left((P_{i,j})_{1,1}^2, \dots, (P_{i,j})_{s,s}^2\right)$, so each entry on the diagonal has to be either zero or one.
Since for each $i \in \{1, \dots, n\} : \sum_{j=1}^n P_{i,j} = \mathrm{I}_s$ it holds that for all $\ell \in \{1, \dots, s\}$ there exists a unique $j \in \{1, \dots, n\}$ such that$(P_{i,j})_{\ell,\ell} = 1$.
For $i \in \{1, \dots, s\},\ \ell, k \in \{1, \dots, n\}$ we set

$$A_{\ell,k}^{(i)} := \begin{cases} e_1 & \text{if } (P_{l,k})_{i,i} = 1 \\ e_j & \text{else} \end{cases}.$$

where $e_1, \dots, e_n \in \mathbb{C}^n$ is the standard basis and $j \neq 1$ is chosen in a way, such that $A^{(i)}$ is a quantum Latin square for each i. By the above reasoning, we are always able to do so. Since we only use one orthonormal basis, we even get $\left(A_{\ell,k}^{(i)} A_{\ell,k}^{(i)^*}\right)_{\ell,k} \in \mathcal{L}_n$.
Next, for $i \in \{1, \dots, s\}$, we define $V_i^* = (e_i^{(s)}|0 \dots 0) \in \mathrm{Mat}_{s,n}(\mathbb{C})$ as the matrix with 1 in the $(i,1)$-th component and 0 everywhere else.
Then

$$V_i^* A_{\ell,k}^{(i)} = \begin{cases} V_i^* e_1 & \text{if } (P_{\ell,k})_{i,i} = 1 \\ V_i^* e_j & \text{else} \end{cases} = \begin{cases} e_i & \text{if } (P_{\ell,k})_{i,i} = 1 \\ 0 & \text{else} \end{cases}.$$

Therefore we have

$$\sum_{i=1}^s V_i^* A_{l,k}^{(i)} A_{l,k}^{(i)^*} V_i = \sum_{i=1}^s \delta_{(P_{\ell,k})_{i,i},1} e_i e_i^* = P_{l,k}.$$

It also holds that $\sum_{i=1}^s V_i^* V_i = \sum_{i=1}^s e_i e_i^* = \mathrm{I}_s$. Therefore $P \in mconv(\mathcal{L}_n)$.
Now let $B \in \mathcal{CP}_s^{(n)}$ be arbitrary. Then we know that all $B_{i,j}$ are hermitian and projectors, hence normal. By the definition of $\mathcal{CP}^{(n)}$ we get that all the $B_{i,j}$ commute. Therefore we can diagonalize all these matrices simultaneously by one unitary $U \in \mathrm{Mat}_{s,s}(\mathbb{C})$:

$$\forall i, j \in \{1, \dots, s\} : U B_{i,j} U^* = \operatorname{diag}(\lambda_{i,j}^{(1)}, \dots, \lambda_{i,j}^{(s)})$$

where $\lambda_{i,j}^{(1)}, \dots, \lambda_{i,j}^{(s)}$ are the eigenvalues of $B_{i,j}$.
Since $B_{i,j}$ are positive semi-definite matrices, all the eigenvalues are greater or equal to 0. Because $U B_{i,j} U^*$ is still a projector, we get $\lambda_{i,j}^{(k)} \in \{0, 1\}$ for all applicable i, j, k.
Now $(U B_{i,j} U^*)_{i,j=1}^s$ is still a quantum magic square, since U is unitary. Therefore, we can apply the previous result and get matrices V_i and quantum Latin squares $A^{(i)}$ like above.

Next, we set $\tilde{V}_i = V_i U$. Then

$$\begin{aligned}\sum_{i=1}^{s} \tilde{V}_i^* A_{\ell,k}^{(i)} {A_{\ell,k}^{(i)}}^* \tilde{V}_i &= \sum_i U^* V_i^* A_{\ell,k}^{(i)} {A_{\ell,k}^{(i)}}^* V_i U \\ &= U^* \left(\sum_i V_i^* A_{\ell,k}^{(i)} {A_{\ell,k}^{(i)}}^* V_i \right) U = U^* U B_{\ell,k} U^* U = B_{\ell,k}\end{aligned}$$

Also note that $\sum_{i=1}^{s} \tilde{V}_i^* \tilde{V}_i = U^* \left(\sum_i V_i^* V_i\right) U = \mathrm{I}_s$. Hence we have shown $B \in mconv(\mathcal{L}_n)$. Since B was chosen arbitrarily this gives the desired result. $\square$

Finally, we can put all the previous results together to see that any quantum magic square that uses a classical Latin square in its construction will be semiclassical.

Corollary 4.14. For all $n \in \mathbb{N}$ it holds that

$$\mathcal{SC}^{(n)} = mconv(\mathcal{CP}^{(n)}) = mconv(\mathcal{L}_n) = mconv(\mathcal{PVMLS}^{(n)}) = mconv(\mathcal{POVMLS}^{(n)}).$$

Proof. The first equality was shown in Theorem 2.37, the second equality follows from Theorem 4.13 and the third equality was proven in Theorem 4.12. The last equality was shown in Proposition 4.11. $\square$

Remark 4.15. We know that $\mathcal{L}_n \subseteq \mathcal{RO}_n^{(n)}$ hence $\mathcal{SC}^{(n)} = mconv(\mathcal{L}_n) \subseteq mconv(\mathcal{RO}_n^{(n)})$ directly follows. This inclusion is, for $n = 4$, a proper inclusion. To see this, consider the quantum Latin square from Example 3.3 (2) :

$$L = \begin{array}{|c|c|c|c|}\hline v_1 & v_2 & v_3 & v_4 \\ \hline \frac{1}{\sqrt{2}}(v_2 - v_3) & \frac{1}{\sqrt{5}}(iv_1 + 2v_4) & \frac{1}{\sqrt{5}}(2v_1 + iv_4) & \frac{1}{\sqrt{2}}(v_2 + v_3) \\ \hline \frac{1}{\sqrt{2}}(v_2 + v_3) & \frac{1}{\sqrt{5}}(2v_1 + iv_4) & \frac{1}{\sqrt{5}}(iv_1 + 2v_4) & \frac{1}{\sqrt{2}}(v_2 - v_3) \\ \hline v_4 & v_3 & v_2 & v_1 \\ \hline \end{array}$$

After embedding this quantum Latin square into our setting of quantum magic squares as described in Proposition 4.1 it will not be in $\mathcal{CP}_4^{(4)}$ since for example the $(1,1)$ and $(2,2)$ entries do not commute:

$$L_{1,1}L_{1,1}^* L_{2,2} L_{2,2}^* = v_1 v_1^* \frac{1}{\sqrt{5}}(iv_1 + 2v_4) \left(\frac{1}{\sqrt{5}}(iv_1 + 2v_4) \right)^* = \frac{1}{5}(v_1 v_1^* + 2iv_1 v_4^*)$$

$$L_{2,2}L_{2,2}^* L_{1,1} L_{1,1}^* = \frac{1}{\sqrt{5}}(iv_1 + 2v_4) \left(\frac{1}{\sqrt{5}}(iv_1 + 2v_4) \right)^* v_1 v_1^* = \frac{1}{5}(v_1 v_1^* - 2iv_4 v_1^*)$$

If we for example choose the v_i to be the standard basis of $\mathbb{C}^4$ then $2iv_1v_4^* \neq -2iv_4v_1^*$ and hence the with L associated quantum magic square $\tilde{L}$ is in $\mathcal{RO}_4^{(4)} \setminus \mathcal{CP}_4^{(4)} \subseteq \mathcal{P}_4^{(4)} \setminus \mathcal{CP}_4^{(4)}$. By the argument given in the proof of Corollary 2.40 $\tilde{L} \notin \mathcal{SC}_4^{(4)} = mconv(\mathcal{L}_4)$.
For even $n = 2k \geq 4$ we can use the following argument. Let L be a classical

Latin square of size $\frac{n}{2}$ and let $a_1, \dots, a_{n/2} \in \mathbb{C}^{n/2},\ b_1, \dots, b_{n/2} \in \mathbb{C}^{n/2}$ be two orthonormal bases such that $a_1 a_1^* b_1 b_1^* \neq b_1 b_1^* a_1 a_1^*$. Let $A, B \in \mathcal{L}_{n/2}$ be the quantum magic squares generated by L and $a_1, \dots, a_{n/2} \in \mathbb{C}^{n/2},\ b_1, \dots, b_{n/2} \in \mathbb{C}^{n/2}$ respectively. The following block matrix like combination of the two is a quantum permutation matrix of size n.

$$A \tilde{\oplus} B := \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \in \mathcal{P}^{(n)}$$

For example, for $n = 4$ this would be the matrix

$$\begin{pmatrix} a_1 a_1^* & a_2 a_2^* & 0 & 0 \\ a_2 a_2^* & a_1 a_1^* & 0 & 0 \\ 0 & 0 & b_1 b_1^* & b_2 b_2^* \\ 0 & 0 & b_2 b_2^* & b_1 b_1^* \end{pmatrix}$$

By our choice of the bases, we have that $A \tilde{\oplus} B \notin \mathcal{CP}^{(n)}$. Hence the argument in the proof of Corollary 2.40 (2) shows that $A \tilde{\oplus} B \notin \mathcal{SC}^{(n)}$.
But $A \tilde{\oplus} B \in mconv(\mathcal{RO}_n^{(n)})$ which we can see as follows. Let

$$\iota : \mathbb{C}^{n/2} \to \mathbb{C}^n : v \mapsto \begin{pmatrix} v_1 \\ \vdots \\ v_{n/2} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

and $e_1, \dots, e_n \in C^n$ the standard basis, i.e. e_k has entry 1 at the k-th position and zeros everywhere else. Let $E_{i,j} = e_{L_{i,j}+n/2}\ e^*_{L_{i,j}+n/2}$ and hence $E = (E_{i,j})_{i,j=1}^{n/2}$ is basically the quantum magic square generated by L and $e_{n/2+1}, \dots, e_n$, but not quite since those vectors do not directly form an orthonormal basis of $\mathbb{C}^{n/2}$. Let $\iota(A) = (\iota(a_{L_{i,j}})\iota(a_{L_{i,j}})^*)_{i,j}$ denote the componentwise application of ι, then

$$C = \begin{pmatrix} \iota(A) & E \\ E & \iota(B) \end{pmatrix} \in \mathcal{RO}_n^{(n)}$$

since all entries have rank one and each row and each column sums over the rank one squares of an orthonormal basis of $\mathbb{C}^n$ and these sums equal the identity. For $n = 4$ this looks like

$$\begin{pmatrix} \iota(a_1)\iota(a_1)^* & \iota(a_2)\iota(a_2)^* & e_3 e_3^* & e_4 e_4^* \\ \iota(a_2)\iota(a_2)^* & \iota(a_1)\iota(a_1)^* & e_4 e_4^* & e_3 e_3^* \\ e_3 e_3^* & e_4 e_4^* & \iota(b_1)\iota(b_1)^* & \iota(b_2)\iota(b_2)^* \\ e_4 e_4^* & e_3 e_3^* & \iota(b_2)\iota(b_2)^* & \iota(b_1)\iota(b_1)^* \end{pmatrix}$$

Set $V = \begin{pmatrix} \mathrm{I}_{n/2} \\ 0 \end{pmatrix} \in \mathrm{Mat}_{n,n/2}(\mathbb{C})$. Then $V^*V = \mathrm{I}_{n/2}$ and

$$\begin{aligned} V^*\iota(a_k)\iota(a_k)^*V &= a_k a_k^* \\ V^* e_k e_k^* V &= 0 \text{ for } k > n/2 \end{aligned}$$

Thus we get $V^*CV = A\tilde{\oplus}B \in mconv(\mathcal{RO}_n^{(n)}) \setminus \mathcal{SC}^{(n)}$.
Since $\mathcal{SC}^{(n)}$ is matrix convex, this also implies that $\mathcal{SC}_n^{(n)} \subsetneq \mathcal{RO}_n^{(n)}$.
For odd n, we cannot use this construction, since the zero blocks in $A\tilde{\oplus}B$ are not square, hence we cannot fill them with some slightly altered embedded Latin square. It seems very likely that we need to use a different approach for odd n, but it is not clear what this approach could be.

5 Arveson Extreme Points

For convex sets we introduced the notion of extreme points (Definition 2.8). A point in the convex set is an extreme point if it cannot be written as convex combination of two different points from the set. In this section we will generalize the notion of extreme points to matrix convex sets.
We will follow the definition in [9] but again adjust it to our setting of $\mathrm{Mat}_n(\mathrm{Mat}_s(\mathbb{C}))$ instead of the original setting in $(\mathrm{Mat}_s(\mathbb{C}))^n$.

Definition 5.1. Let $R = \bigcup_{s\in\mathbb{N}} R_s$ be a matrix convex set as defined in 2.23. $A = (A_{i,j})_{i,j=1}^n \in R_s$ is called **Arveson extreme point** of R if R does not contain a nontrivial dilation of A. That means if there exist $B = (B_{i,j})_{i,j} \in \mathrm{Mat}_n(\mathrm{Mat}_{s,t}(\mathbb{C}))$, $C = (C_{i,j})_{i,j} \in \mathrm{Mat}_n(\mathrm{Her}_t(\mathbb{C}))$ such that

$$D = \left(\begin{pmatrix} A_{i,j} & B_{i,j} \\ (B^*)_{i,j} & C_{i,j} \end{pmatrix} \right)_{i,j=1}^n \in R_{s+t}$$

then $B = 0$ has to hold.
Note that D is called a dilation of A.

If a matrix convex set is a so called compact free spectrahedron, which means that it is generated by matrix inequalities, then the matrix convex hull of its Arveson extreme points already gives the whole set. This was shown in [9].

Definition 5.2. Given some hermitian matrices $A_{i,j} \in \mathrm{Her}_d(\mathbb{C})$, $i,j \in \{1,\dots,n\}$. The s-level of the **free spectrahedron** generated by the $A_{i,j}$ is

$$FS((A_{i,j})_{i,j=1}^n)_s = \left\{ X \in \mathrm{Mat}_n(\mathrm{Her}_s(\mathbb{C})) \mid \mathrm{I}_d \otimes \mathrm{I}_s + \sum_{i,j=1}^n A_{i,j} \otimes X_{i,j} \geq 0 \right\}$$

As usual, the free spectrahedron is the union over all its levels.

A matrix convex set $R = \bigcup_{s\in\mathbb{N}} R_s$ is compact if

- it is bounded, i.e. there exists a constant $c \in \mathbb{R},\ c > 0$ such that for all $s \in \mathbb{N}$ and all $X \in R_s$ we have

$$c\,\mathrm{I}_s - \sum_{i,j} X_{i,j}^2 \geq 0.$$

- it is closed, meaning that each level is closed.

The notion of free spectrahedron is again a generalization from classical geometry to the free/non-commutative setting.
Every free spectrahedron is clearly a matrix convex set.

Theorem 5.3. Every compact free spectrahedron is the matrix convex hull of its Arveson extreme points.

The proof of this theorem can be found in [9], Theorem 1.1.

Next, we will see a nice result that classifies the Arveson extreme points of the set of quantum magic squares. This is again taken from [8].

Corollary 5.4. Every quantum permutation matrix is an Arveson extreme point of the matrix convex set $\mathcal{M}^{(n)}$ of all quantum magic squares.
For $n \geq 3$ not every Arveson extreme point is a quantum permutation matrix.

Proof. Let $U = (U_{i,j})_{i,j} \in \mathcal{P}_s^{(n)}$ and assume there is a quantum magic square $A \in \mathcal{M}_t^{(n)}$ and an isometry $V \in \mathrm{Mat}_{t,s}(\mathbb{C})$ such that $U = (V^* A_{i,j} V)_{i,j}$.
Then $0 \leq A_{i,j} \leq \mathrm{I}_t$, since A is a quantum magic square. Lemma 2.39 gives that, up to basis change,

$$A_{i,j} = \begin{pmatrix} U_{i,j} & 0 \\ 0 & P_{i,j} \end{pmatrix}$$

for some $P_{i,j} \in \mathrm{Her}_{t-s}(\mathbb{C})$. But this just means that the dilation was trivial, hence U is an Arveson extreme point.

On the other hand, we know that for $n \geq 3$ we have $mvonc(\mathcal{P}^{(n)}) \neq \mathcal{M}^{(n)}$.
$\mathcal{M}^{(n)}$ is a compact free spectrahedron, which we can see as follows:
First, we need to shift the set of quantum magic squares to contain the all zero matrix, since it is contained in any free spectrahedron in the way we defined it.
Hence, we look at

$$\widetilde{\mathcal{M}}^{(n)} = \left\{ \left(A_{i,j} - \frac{1}{n}\,\mathrm{I} \right)_{i,j} \mid A = (A_{i,j})_{i,j} \in \mathcal{M}^{(n)} \right\}$$

Then $\widetilde{\mathcal{M}}^{(n)}$ is defined by the following matrix inequalities:

$B = (A_{i,j} - \frac{1}{n}\,\mathrm{I})_{i,j} \in \widetilde{\mathcal{M}}^{(n)}$ if and only if

$$\begin{aligned}
\forall i,j \in \{1,\dots,n\} :\ & \mathrm{I} + nB_{i,j} \geq 0 \\
\forall j \in \{1,\dots,n\} :\ & \sum_{i=1}^{n} B_{i,j} \geq 0 \\
\forall j \in \{1,\dots,n\} :\ & \sum_{i=1}^{n} -B_{i,j} \geq 0 \\
\forall i \in \{1,\dots,n\} :\ & \sum_{j=1}^{n} B_{i,j} \geq 0 \\
\forall i \in \{1,\dots,n\} :\ & \sum_{j=1}^{n} -B_{i,j} \geq 0.
\end{aligned}$$

This holds, because:

$$\begin{aligned}
\mathrm{I} + nB_{i,j} \geq 0 &\iff nA_{i,j} \geq 0 \iff A_{i,j} \geq 0 \\
\sum_{i=1}^{n} B_{i,j} \geq 0 &\iff \left(\sum_{i=1}^{n} A_{i,j}\right) - \mathrm{I} \geq 0 \\
\sum_{i=1}^{n} -B_{i,j} \geq 0 &\iff \mathrm{I} - \left(\sum_{i=1}^{n} A_{i,j}\right) \geq 0 \\
\sum_{j=1}^{n} B_{i,j} \geq 0 &\iff \left(\sum_{j=1}^{n} A_{i,j}\right) - \mathrm{I} \geq 0 \\
\sum_{j=1}^{n} -B_{i,j} \geq 0 &\iff \mathrm{I} - \left(\sum_{j=1}^{n} A_{i,j}\right) \geq 0.
\end{aligned}$$

These inequalities can be encoded into one large block matrix to get one matrix inequality in the form of the free spectrahedron.
The set of quantum magic squares is closed, since it is defined by closed conditions only. It is bounded, since all rows and columns sum to the identity, therefore the sum over all entries of a quantum magic square will be n times the identity.

Thus, Theorem 5.3 and Theorem 2.41 give that there must be more Arveson extreme points then just the permutation matrices.

□

Lemma 5.5. For $X \in \mathcal{POVMLS}^{(n)}$ the following are equivalent

(1) X is an Arveson extreme point in $\mathcal{M}^{(n)}$

(2) X is an Arveson extreme point in $\mathcal{SC}^{(n)}$

Proof. (1) $\Rightarrow$ (2): If X has no nontrivial dilation in $\mathcal{M}^{(n)}$ it cannot have a nontrivial dilation in $\mathcal{SC}^{(n)} \subseteq \mathcal{M}^{(n)}$.
(2) $\Rightarrow$ (1): Let $\begin{pmatrix} X & \beta \\ \beta^* & \gamma \end{pmatrix}$ be a nontrivial dilation of X in $\mathcal{M}^{(n)}$, i.e. for some $\ell \in \mathbb{N}$ we have $0 \neq \beta_{i,j} \in \mathrm{Mat}_{n,\ell}(\mathbb{C})$, $\gamma_{i,j} \in \mathrm{PSD}_\ell$ such that

$$\left(\begin{pmatrix} X_{i,j} & \beta_{i,j} \\ \beta_{i,j}^* & \gamma_{i,j} \end{pmatrix}\right)_{i,j=1}^{n} \in \mathcal{M}_{s+\ell}^{(n)}.$$

Per definition, X is generated by a Latin square L of size n and a POVM $P_1, \ldots, P_n$. For $k = 1, \ldots, n$ set

$$(L_k)_{i,j} = \begin{cases} 1 & \text{if } L_{i,j} = k \\ 0 & \text{else} \end{cases}$$

Then, analogously to the proof of Lemma 4.9, we get the representation

$$X = \sum_k L_k \otimes P_k.$$

For every $k \in \{1, \ldots, n\}$ we can find a $j_k \in \{1, \ldots, n\}$ such that $L_{1,j_k} = k$, i.e. j_k is the unique position of k in the first row of the Latin square L. Note that each number from $\{1, \ldots, n\}$ will appear exactly once as one of the j_k's.
Setting

$$q_k = \begin{pmatrix} P_k & \beta_{1,j_k} \\ \beta_{1,j_k}^* & \gamma_{1,j_k} \end{pmatrix}$$

we get that

$$0 \leq \begin{pmatrix} X_{1,j_k} & \beta_{1,j_k} \\ \beta_{1,j_k}^* & \gamma_{1,j_k} \end{pmatrix} = \begin{pmatrix} P_k & \beta_{1,j_k} \\ \beta_{1,j_k}^* & \gamma_{1,j_k} \end{pmatrix} = q_k$$

and

$$\begin{aligned} \sum_{k=1}^{n} q_k &= \begin{pmatrix} \sum_{k=1}^n P_k & \sum_{k=1}^n \beta_{1,j_k} \\ \sum_{k=1}^n \beta_{1,j_k}^* & \sum_{k=1}^n \gamma_{1,j_k} \end{pmatrix} = \begin{pmatrix} \sum_{k=1}^n P_k & \sum_{j=1}^n \beta_{1,j} \\ \sum_{j=1}^n \beta_{1,j}^* & \sum_{k=1}^n \gamma_{1,j} \end{pmatrix} \\ &= \sum_{j=1}^{n} \begin{pmatrix} X_{1,j} & \beta_{1,j} \\ \beta_{1,j}^* & \gamma_{1,j} \end{pmatrix} = \mathrm{I}_{s+\ell}\,. \end{aligned}$$

Hence $Q = \sum_k L_k \otimes q_k \in \mathcal{SC}_{s+\ell}^{(n)}$ is a nontrivial dilation of X in $\mathcal{SC}^{(n)}$. $\square$

Corollary 5.6. From paper [8] we know that every element from $\mathcal{P}^{(n)}$ is an Arveson extreme point in $\mathcal{M}^{(n)}$. This implies that every element from $\mathcal{SC}^{(n)} \cap \mathcal{P}^{(n)}$ is an Arveson extreme point of $\mathcal{SC}^{(n)}$.

Remark 5.7. The cone of non-normalized magic squares $\mathcal{C}^{(n)}$ (Definition 2.28) is not a simplex cone (Lemma 2.29). Hence $\mathcal{S}^{(n)}$, the smallest operator system over $\mathcal{C}^{(n)}$ is not a free spectrahedral cone by Theorem 4.7 in [10].
On the other hand we have that $\mathcal{SC}^{(n)} = \mathcal{S}^{(n)} \cap \mathcal{M}^{(n)}$. Can we conclude from this that $\mathcal{SC}^{(n)}$ is not a free spectrahedron?

6 Appearances of Quantum Magic Squares in other Contexts

In this section, we will examine different topics in which quantum magic squares appear. We summarize these topics and give a short idea of how one can look at these different topics from our view of quantum magic squares. This section will only scrape the surface of what might be possible.

6.1 Orthogonal Quantum Latin Squares

The notion of orthogonal quantum Latin squares became known when Leonhard Euler stated the thirty-six officers problem:
Can one arrange 36 officers from six regiments with six different ranks in a 6×6 square such that in each row and column there is exactly one officer from each regiment and each rank?
This translates to the setting of Latin squares in the following way:
Do there exist two Latin squares of size 6 A, B such that no two pairs $(A_{i,j}, B_{i,j})$ are the same for $1 \leq i, j \leq 6$?
Euler already suspected that the answer to his question was "no", but it was only proven by G. Terry in the year 1900 [28].
Of course the question arises how one can generalize this problem to the quantum setting. There are several definitions of orthogonal quantum Latin squares, the probably most intuitive one by Musto and Vicary was given in [20]. They showed that it is equivalent to another definition given in [11].

Definition 6.1. Two quantum Latin squares $A = (A_{i,j})_{i,j}, B = (B_{i,j})_{i,j} \in \mathrm{Mat}_n(\mathbb{C}^n)$ are called orthogonal if $\{A_{i,j} \otimes B_{i,j} \mid i, j \in \{1, \dots, n\}\}$ forms an orthonormal basis of $\mathbb{C}^n \otimes \mathbb{C}^n \cong \mathbb{C}^{n^2}$

In [26] they use a slightly different definition that allows the two quantum Latin squares to be entangled.

Definition 6.2. Consider $\psi_{i,j} \in \mathbb{C}^d \otimes \mathbb{C}^d$ of norm one for all $i, j \in \{1, \dots, d\}$. Then $\psi_{i,j} = \sum_{k,\ell=1}^{d} C_{k,\ell}^{i,j} e_k \otimes e_\ell$ for some $C_{k,\ell}^{i,j} \in \mathbb{C}$. $(\psi_{i,j})_{i,j=1}^{d}$ is an orthogonal quantum Latin square if

(1) $\psi_{i,j}^* \psi_{k,\ell} = \delta_{i,k}\delta_{j,\ell}$

(2) $\mathcal{C} := (C^{i,j})_{i,j=1}^{d} \in \mathrm{Mat}_d(\mathrm{Mat}_d(\mathbb{C}))$ satisfies

  (a) $\sum_{i=1}^{d} C^{i,j} \left(C^{i,\ell}\right)^* = \delta_{j,\ell} \, \mathrm{I}_d$

  (b) $\sum_{j=1}^{d} C^{i,j} \left(C^{k,j}\right)^* = \delta_{i,k} \, \mathrm{I}_d$

Proposition 6.3. If two quantum Latin squares A, B are orthogonal in the sense of Definition 6.1 then $(A_{i,j} \otimes B_{i,j})_{i,j}$ is an orthogonal quantum Latin square in the sense of Definition 6.2.

Proof. Let A, B be two quantum Latin squares of size n that are orthogonal. Set $\psi_{i,j} = A_{i,j} \otimes B_{i,j}$.
Then it directly follows that $(\psi_{i,j})_{i,j}$ satisfies condition (1) of Definition 6.2.
Two check condition (2), let $e_1, \ldots, e_n \in \mathbb{C}^n$ denote the standard basis of $\mathbb{C}^n$. We have the following representations with respect to this basis:

$$A_{i,j} = \sum_{k=1}^{n} \lambda_k^{i,j} e_k, \;\; B_{i,j} = \sum_{k=1}^{n} \gamma_k^{i,j} e_k \text{ for all } i, j \in \{1, \ldots, n\}.$$

Hence for any $i, j \in \{1, \ldots, n\}$ we have

$$\psi_{i,j} = \left(\sum_{k=1}^{n} \lambda_k^{i,j} e_k\right) \otimes \left(\sum_{\ell=1}^{n} \gamma_\ell^{i,j} e_\ell\right) = \sum_{k,\ell} \lambda_k^{i,j} \gamma_\ell^{i,j} (e_k \otimes e_\ell).$$

Thus $C_{k,\ell}^{i,j} = \lambda_k^{i,j} \gamma_\ell^{i,j}$ and $C^{i,j} = \sum_{k,\ell} C_{k,\ell}^{i,j} e_k e_\ell^*$. Therefore, for $i, j, d \in \{1, \ldots, n\}$, we have

$$\begin{aligned} C^{i,\ell}(C^{i,d})^* &= \sum_{k,\ell,p,q} C_{k,\ell}^{i,j} e_k e_\ell^* \overline{C_{p,q}^{i,d}} e_q e_p^* = \sum_{k,\ell,p,q} C_{k,\ell}^{i,j} \overline{C_{p,q}^{i,d}} e_k \underbrace{e_\ell^* e_q}_{=\delta_{\ell,q}} e_p^* \\ &= \sum_{k,p} \left(\sum_\ell C_{k,\ell}^{i,j} \overline{C_{p,q}^{i,d}} \right) e_k e_p^* \overset{(*)}{=} \delta_{j,d} \left(\sum_k \lambda_k^{i,j} e_k \right) \left(\sum_p \overline{\lambda_p^{i,d}} e_p^* \right) \\ &= \delta_{j,d} A_{i,j} A_{i,d}^*. \end{aligned}$$

In $(*)$ we use that

$$\sum_\ell C_{k,\ell}^{i,j} \overline{C_{p,q}^{i,d}} = \sum_\ell \lambda_k^{i,j} \gamma_\ell^{i,j} \overline{\lambda_p^{i,d} \gamma_\ell^{i,d}} = \lambda_k^{i,j} \overline{\lambda_p^{i,d}} \sum_\ell \gamma_\ell^{i,j} \overline{\gamma_\ell^{i,d}} = \lambda_k^{i,j} \overline{\lambda_p^{i,d}} B^{i,q^*} B^{i,j} = \lambda_k^{i,j} \overline{\lambda_p^{i,d}} \delta_{j,d}.$$

And hence

$$\sum_{i=1}^{n} C^{i,j} (C^{i,\ell})^* = \delta_{j,\ell} \sum_{i=1}^{n} A_{i,j} A_{i,j}^* = \delta_{j,\ell} \, \mathrm{I}_n$$

where we used Proposition 4.1 for the last equality.
This shows that the $\psi_{i,j}$ satisfy condition (2a) of Definition 6.2. Condition (2b) follows from an analogues argument for the columns. $\square$

Remark 6.4. (1) A quantum state $\psi \in \mathbb{C}^n \otimes \mathbb{C}^n$ is called separable if it can be written as $\psi = a \otimes b$ for some $a, b \in \mathbb{C}^n$. If it is not separable, we call it entangled.
In this framework we can understand the difference of the Definitions 6.1 and 6.2 in the way that in Definition 6.1 all entries of the orthogonal quantum Latin square are separable, while Definition 6.2 allows for entanglement between the two quantum Latin squares.

(2) If we have an orthogonal quantum Latin square in the sense of Definition 6.2 and set $B_{i,j} = C^{i,j}(C^{i,j})^*$ then $B = (B_{i,j})_{i,j}$ is a quantum magic

square. This directly follows from condition (2) in the definition.
Condition (1) implies that $\operatorname{tr}(B_{i,j}) = 1$ for all i, j since

$$\psi_{i,j}^* \psi_{k,\ell} = \sum_{p,q} \overline{C_{p,q}^{i,j}} C_{p,q}^{k,\ell} = \operatorname{tr}(C^{k,\ell}(C^{i,j})^*).$$

Hence B will be some very special quantum magic square.
It might be interesting to further investigate the class of quantum magic squares that arise in this way and maybe find a way to construct orthogonal quantum Latin squares from quantum magic squares.

Orthogonal quantum Latin squares are closely related to absolutely maximally entangled states and 2-unitary matrices which play important roles in quantum computation. More details can be found in [26].
In this paper the authors solve an open problem of quantum information theory as stated in [16]: They show that there exist "36 entangled officers", i.e. there is an orthogonal quantum Latin square of size 6.
Once again the quantum version can achieve more than its classical counterpart.

6.2 SudoQ

The classical Sudoku puzzle is a 9×9 square with some blank entries that has to be filled with the numbers from 1 to 9 in such a way that it forms a Latin square with the extra condition that nine 3×3 sub-squares are also filled with the numbers from 1 to 9 each appearing exactly once.
The Sudoku became its quantum version "SudoQ" in [21] by Ion Nechita and Jordi Pillet where they defined:

Definition 6.5. A SudoQ square of size n^2 is a $n^2 \times n^2$ matrix of vectors from $\mathbb{C}^{n^2}$ such that the vectors in each row, column and $n \times n$ sub-square form an orthonormal basis of $\mathbb{C}^{n^2}$.

Any SudoQ square is clearly a quantum Latin square and we can use Proposition 4.1 to treat them as quantum magic squares.
In [21] the authors investigate under what circumstances a SudoQ square, where some entries are left blank, has a solution.
In [22] SudoQs are further investigated. They introduce a notion of apparently classical quantum Latin squares which directly corresponds to our set $\mathcal{L}_n$.
They show that every quantum Latin square of size 3 is apparently classical. In our setting this means $\mathcal{L}_3 = \mathcal{RO}_3^{(3)}$. This also follows from our results:
Remark 2.18 says that $\mathcal{CP}^{(3)} = \mathcal{P}^{(3)}$, Remark 4.3 gives $\mathcal{L}_n \subseteq \mathcal{CP}^{(n)}$, $\mathcal{RO}^{(n)} \subseteq \mathcal{P}^{(n)}$ and Proposition 4.4 tell us $\mathcal{SC}^{(n)} \cap \mathcal{RO}_n^{(n)} = \mathcal{L}_n$. Together we get that $\mathcal{P}^{(3)} \subseteq \mathcal{SC}^{(3)}$ and hence

$$\mathcal{L}_3 = \mathcal{SC}^{(3)} \cap \mathcal{RO}_3^{(3)} = \mathcal{RO}_3^{(3)}.$$

6.3 Quantum (Permutation) Groups

In this part we will take a look at quantum groups and especially quantum permutation groups to see how these objects are related to quantum magic squares.
We will need some theoretical background. Here we will just give a quick revision of the relevant notions following [2], Chapter 1.

Theorem 6.6. Given a compact topological space X (i.e. a set equipped with some topology such that every open cover of X has a finite subcover), $C(X)$ is the $\mathbb{C}$-algebra of continuous functions $f : X \to \mathbb{C}$ with pointwise addition and multiplication. Then $C(X)$ is a C^*-algebra with norm and involution given by

$$\|f\| = \sup_{x \in X} |f(x)|$$
$$f^*(x) = \overline{f(x)}.$$

This algebra is commutative and any commutative C^*-algebra is of this form.

The proof of this theorem can be found in [2], Theorem 1.4.
In this case X is called a compact quantum space. Even when given an arbitrary (non-commutative) C^*- algebra A, we will write $A = C(X)$ and call X compact quantum space.
To construct the quantum permutation group S_N^+, let us first consider S_N, the group of permutations of N elements. Define the mappings $u_{i,j} : S_N \to \mathbb{C}$ by

$$u_{i,j}(\pi) = \begin{cases} 1 & \text{if } \pi(i) = j \\ 0 & \text{else} \end{cases}.$$

$u_{i,j}(\pi)$ can also be seen as the projection onto the i, j-th entry of the permutation matrix corresponding to π.
Then $u_{i,j} \in C(S_N)$ is a projector and $u = (u_{i,j})_{i,j=1}^N$ is a quantum permutation matrix over the C^*-algebra $C(S_N)$, since the entries in each row and each column will sum to the constant one map, the identity in $C(S_N)$.
On the other hand, the relations that u satisfies are enough to generate $C(S_N)$ as a universal commutative C^*-algebra. That is, it is given by a set of generators, here $\{u_{i,j}\}_{i,j=1}^N$ and a set of relations, namely that $u = (u_{i,j})_{i,j}$ forms a quantum permutation matrix (although more in an abstract sense, not over one specific C^* algebra).

$$C(S_N) = C^*_{comm}\left(\{u_{i,j}\}_{i,j=1}^N \mid u \text{ is abstract quantum permutation matrix }\right)$$

By generating a C^*-algebra that is not commutative anymore, we get to the quantum permutation group.

Theorem 6.7. The universal C^*-algebra

$$C(S_N^+) := C^*\left(\{u_{i,j}\}_{i,j=1}^N \mid u \text{ is abstract quantum permutation matrix }\right)$$

is a Woronowicz algebra with

- comultiplication $\Delta : C(S_N^+) \to C(S_N^+) \otimes C(S_N^+)$ given by

$$\Delta(u_{i,j}) = \sum_k u_{i,j} \otimes u_{k,j}$$

- counit $\varepsilon : C(S_N^+) \to \mathbb{C}$ given by $\varepsilon(u_{i,j}) = \delta_{i,j}$
- antipode $S : C(S_N^+) \to C(S_N^+)$ given by $S(u_{i,j}) = u_{j,i}$.

The underlying compact quantum space S_N^+ is a compact quantum group called quantum permutation group.

The proof of this theorem can be found in [2].

Definition 6.8. A Woronowicz algebra is a C^*-algebra A together with a unitary matrix $u \in \mathrm{Mat}_N(A)$ whose entries generate A and the formulas

$$\Delta(u_{i,j}) = \sum_k u_{i,j} \otimes u_{k,j}$$
$$\varepsilon(u_{i,j}) = \delta_{i,j}$$
$$S(u_{i,j}) = u_{j,i}^*$$

define C^*-homomorphisms

$$\Delta : A \to A \otimes A$$
$$\varepsilon : A \to \mathbb{C}$$
$$S : A \to A^{\text{opposite}}$$

Remark 6.9. (1) That the construction in Theorem 6.7 is a Woronowicz algebra basically only requires that Δ, ε and S are C^*-homomorphisms. Given a compact Lie group G, $C(G)$ is a Woronowicz algebra. In this spirit, given any Woronowicz algebra A we write $A = C(G)$ and call G a compact quantum Lie group.

(2) The notion of Woronowicz algebras is closely related to the notion of Hopf algebras and corepresentations, see for example [24] for more informations on Hopf algebras in this context.

(3) A quantum permutation matrix P of (exterior) size N over some C^*-algebra A gives rise to a representation $\pi : C(S_N^+) \to A$ by defining $\pi(u_{i,j}) = P_{i,j}$.

(4) In [3], Theodor Banica and Ion Necchita have a closer look at these representations given by quantum permutation matrices and also look at what happens when taking different subsets of the quantum permutation matrices, for example $\mathcal{PVMLS}^{(n)}$.
It would be very interesting to further see how our results might be useful in this context, especially how the matrix convex hull could be translated to this setting. Maybe some constructions in [3] could give rise to interesting structures in our setting of quantum magic squares.

6.4 Doubly Normalised Tensor of Positive Semi-Definite Operators

In [12] Leonardo Guerini and Alexandre Baraviera define quantum magic squares under the name Doubly Normalised Tensor of Positive semi-definite Operators (DNT). Their definition goes as follows:

Definition 6.10. Given a Hilbert space $\mathcal{H}$, let $\mathcal{L}(\mathcal{H})$ denote the set of linear operators on $\mathcal{H}$.
A Doubly Normalised Tensor of Positive semi-definite Operators is a tensor $\mathcal{A} \in \mathcal{L}(\mathcal{H})^{n\times n}$ such that each element is positive semi-definite and each column and each row sums up to the identity.
Although not explicitly mentioned in [12], it is most likely that the authors are also taking about bounded linear operators on $\mathcal{H}$. In the finite dimensional case this distinction is not important since then any linear operator will be continuous and hence bounded, but if $\mathcal{H}$ is infinite dimensional, working with possibly unbounded operators would complicate matters significantly.

Next they define the notion of a decomposition into permutation tensors.

Definition 6.11. Given a set of operators $\mathcal{Q} = (Q_j) \in \mathcal{L}(\mathcal{H})^{n!}$ such that each operator is positive semi-definite and $\sum_j Q_j = \mathrm{I}$. Let $P_1, \ldots, P_{n!} \in \mathrm{Mat}_n(\mathbb{C})$ denote all $n \times n$ permutation matrices. Then

$$\sum_{j=1}^{n!} P_j \otimes Q_j$$

is called a decomposition into permutation tensors.

A quantum magic square (or DNT) clearly has a decomposition into permutation tensors if and only if it is semiclassical.
To understand the main theorem of this paper, we need one more definition.

Definition 6.12. A set of POVMs $A^{(j)} = \{A_1^{(j)}, \ldots, A_n^{(j)}\} \subseteq \mathcal{L}(\mathcal{H})$, $j = 1, \ldots, m$ is jointly measurable if there exists a POVM $M = \{M_1, \ldots, M_n\} \subseteq \mathcal{L}(\mathcal{H})$ and a probability distribution μ that gives the probability for $A_j^{(i)}$ given $A^{(i)}$ and M_k, hence it satisfies $\mu(j \mid A^{(i)}, k) \geq 0$ and $\sum_j \mu(j \mid A^{(i)}, k) = 1$ for all i, k, such that

$$A_j^{(i)} = \sum_k \mu(j \mid A^{(i)}, k) M_k.$$

For fixed i and j, this means that $A_j^{(i)}$ is a convex combination of $M_1, \ldots, M_n$.
The main theorem of [12] states:

Theorem 6.13. Let $\mathcal{A} = (A_{i,j})_{i,j=1}^n$ be a DNT and $\mathcal{R} = \{\mathcal{R}^{(i)} = (A_{i,j})_{j=1}^n\}$ the set of all rows of $\mathcal{A}$ and $\mathcal{C} = \{\mathcal{C}^{(j)} = (A_{i,j})_{i=1}^n\}$ the set of all columns of $\mathcal{A}$. Then the following is equivalent for $\mathcal{A}$:

(1) $\mathcal{A}$ admits a decomposition into permutation tensors

(2) (a) $\mathcal{R} \cup \mathcal{C}$ is jointly measurable

(b) μ is symmetric in the sense that for all i, j, k we have

$$\mu(j \mid R^{(i)}, k) = \mu(i \mid C^{(j)}, k).$$

Remark 6.14. This Theorem translates to our setting in the following way. Assume the second condition holds and let M denote the so called mother measure from the joint measurability. Because of the symmetry, we have

$$A_{i,j} = \mathcal{R}_j^{(i)} = \sum_k \mu(j \mid \mathcal{R}^{(i)}, k) M_k = \sum_k \mu(i \mid \mathcal{C}^{(j)}, k) M_k = C_i^{(j)} = A_{i,j}.$$

Hence the symmetry is important for the joint measurability to be meaningful when considering $\mathcal{A}$.
Set $B_{i,j}^{(k)} = \mu(j \mid \mathcal{R}^{(i)}, k) = \mu(i \mid \mathcal{C}^{(j)}, k)$. Then $B^{(k)} = \left(B_{i,j}^{(k)}\right)_{i,j=1}^{n}$ is a magic square since μ was a probability measure.
Since each M_k is positive semi-definite, there exists $V_k \in \mathcal{L}(\mathcal{H})$ such that $M_k = V_k^* V_k$ for all k. We then have

$$A_{i,j} = \sum_k B_{i,j}^{(k)} M_k = \sum_k V_k^* B_{i,j}^{(k)} V_k.$$

We have almost shown that (2) is equivalent to being in $mconv(\mathcal{M}_1^{(n)})$. The only difference is that in the definition of the matrix convex hull we require that the V_k (in this setting) are $\mathrm{Mat}_{1,t}(\mathbb{C})$ if the dimension of $\mathcal{H}$ is t, but so far they are square matrices (if $\mathcal{H}$ is finite dimensional). To overcome this problem, observe that $B_{i,j}^{(k)} \mathrm{I}_t = \sum_\ell e_\ell B_{i,j}^{(k)} e_\ell^*$ and hence $D^{(k)} := \left(B_{i,j}^{(k)} \mathrm{I}_t\right)_{i,j} \in mconv(\mathcal{M}_1^{(n)})$. Thus $A_{i,j} = \sum_k V_k^* B_{i,j}^{(k)} \mathrm{I}_t V_k = \sum_k V_k^* D_{i,j}^{(k)} V_k$ and therefore $A \in mconv(\mathcal{M}_1^{(n)})$. Hence for a finite dimensional Hilbert space $\mathcal{H}$ this theorem is equivalent to Proposition 2.25.

7 Open Questions

In this section we will discuss questions that are still open, go through the difficulties in answering them that have occurred and line out why answers to these questions would be interesting.

7.1 Matrix Convex Hull of the Embedded Quantum Latin Squares

So far, we know that

$$\mathcal{L}_n \subseteq \mathcal{RO}_n^{(n)} \subseteq \mathcal{P}^{(n)}$$

and thus

$$\mathcal{SC}^{(n)} = mconv(\mathcal{L}_n) \subseteq mconv(\mathcal{RO}_n^{(n)}) \subseteq mconv(\mathcal{P}^{(n)}).$$

Several questions arise: Are all these inclusions strict, or do we have equality at some point? Is there a difference between $mconv(\mathcal{RO}_n^{(n)})$ and $mconv(\mathcal{RO}^{(n)})$?

For all easy examples we could think of, the inclusion $\mathcal{P}^{(n)} \subseteq mconv(\mathcal{RO}_n^{(n)})$ holds. For example if $a_1, a_2 \in \mathbb{C}^2$ and $b_1, b_2 \in \mathbb{C}^2$ are two (different) orthonormal bases, then

$$\begin{pmatrix} a_1a_1^* & a_2a_2^* & 0 & 0 \\ a_2a_2^* & a_1a_1^* & 0 & 0 \\ 0 & 0 & b_1b_1^* & b_2b_2^* \\ 0 & 0 & b_2b_2^* & b_1b_1^* \end{pmatrix} \in \mathcal{P}_2^{(4)} \setminus \mathcal{CP}_2^{(4)}$$

is in $mconv(\mathcal{RO}_4^{(4)})$ by taking $\iota : \mathbb{C}^2 \to \mathbb{C}^4 : (a_1, a_2)^T \mapsto (a_1, a_2, 0, 0)^T$. Then

$$\begin{pmatrix} \iota(a_1)\iota(a_1^*) & \iota(a_2)\iota(a_2^*) & e_3e_3^* & e_4e_4^* \\ \iota(a_2)\iota(a_2^*) & \iota(a_1)\iota(a_1^*) & e_4e_4^* & e_3e_3^* \\ e_3e_3^* & e_4e_4^* & \iota(b_1)\iota(b_1^*) & \iota(b_2)\iota(b_2^*) \\ e_4e_4^* & e_3e_3^* & \iota(b_2)\iota(b_2^*) & \iota(b_1)\iota(b_1^*) \end{pmatrix} \in \mathcal{RO}_4^{(4)}$$

is a dilation of the original quantum magic square in $\mathcal{RO}_4^{(4)}$. Hence the original one is in $mconv(\mathcal{RO}_4^{(4)})$.
But the problem here might lie in coming up with more complicated quantum magic squares in $\mathcal{P}^{(n)} \setminus \mathcal{CP}^{(n)}$.
This problem is also closely related with the open question of whether $\mathcal{SC}^{(n)} = mconv(\mathcal{RO}_n^{(n)})$ for odd n in Remark 4.15.

On the other hand, if $mconv(\mathcal{RO}_n^{(n)}) = mconv(\mathcal{P}^{(n)})$, then $mconv(\mathcal{P}^{(n)})$ would only be generated by the level of quantum magic squares where interior and exterior sizes are equal. This would limit the structure of quantum permutation matrices significantly and might have impact on the theory of quantum permutation groups. Therefore, it seems unlikely that equality holds.

7.2 Arveson Extreme Points

First of all, it would be interesting to find the remaining Arveson extreme points of $\mathcal{M}^{(n)}$. This would tell us a great deal about the structure of the set of quantum magic squares. The problem here is mainly where to start. Which type of quantum magic squares might have the potential to also be an Arveson extreme point? This is not clear.
As mentioned in Remark 5.7, it would be interesting to see whether $\mathcal{SC}^{(n)}$ is a free spectrahedron or not. At the moment it seems very likely that it is not since, as described in Remark 5.7, $\mathcal{S}^{(n)}$ the smallest operator system over $\mathcal{C}^{(n)}$ is not a free spectrahedral cone and $\mathcal{SC}^{(n)} = \mathcal{S}^{(n)} \cap \mathcal{M}^{(n)}$.

7.3 From Quantum Magic Squares to Quantum Latin Squares

It would be very useful to have a way to construct quantum Latin squares and/or orthogonal quantum Latin squares from quantum magic squares. Then we could use quantum magic squares to construct unitary error bases, but maybe there is also a more direct way to use quantum magic squares for such constructions. If we can see which properties the quantum magic squares corresponding to orthogonal quantum Latin squares have, we might get more insight into the structure of quantum magic squares. But also, we could probably go from quantum magic squares back to orthogonal quantum Latin squares which might lead to the construction of new absolutely maximally entangled states.

7.4 Connection to Quantum Permutation Groups

Are there ways to use our results in the setting of quantum permutation groups similar to the work in [3]? Is there a way in which the matrix convex hull has a meaning in the setting of quantum permutation matrices?
If we had answers to these questions, a positive answer to whether $\mathcal{P}^{(n)} \subseteq mconv(\mathcal{RO}_n^{(n)})$ might have some impact, since this could lead to simpler/different representations of quantum permutation groups.

8 Conclusion

Generalizing classical structures by using non-commutative objects related to quantum theory gives rise to new, fascinating structures with interesting properties. Quantum magic squares are not given as the matrix convex hull of quantum permutation matrices, as a generalization of Birkhoff-von Neumann's Theorem would suggest.

The set of semiclassical quantum magic squares can be classified nicely: it is the matrix convex hull of the quantum permutation matrices with permuting entries. But also every other quantum magic square that arises from any of our constructions that involve classical Latin squares is semiclassical.

Quantum Latin squares also truly give more structure than classical Latin squares and give a new method to construct unitary error bases, the so called quantum shift-and-multiply method.

We constructed a natural way to embed quantum Latin squares into the setting of quantum magic squares by taking the rank one square of each entry. On the other hand, any quantum magic square where each entry has rank 1 comes from a quantum Latin square. And this embedding is nicely compatible with the notion of semiclassical quantum magic squares.

But a lot of questions are still open. We were only able to show that the matrix convex hull of the rank 1 quantum magic squares of even size is strictly larger then the set of semiclassical quantum magic squares. It is not clear whether this also holds for odd sizes. On the other hand, we were not able to show that the matrix convex hull of the quantum permutation matrices is strictly larger than the matrix convex hull of the rank 1 quantum magic squares. This question would be very interesting to solve as it might also have impact on the theory of quantum permutation groups.

We saw that the quantum permutation matrices are Arveson extreme points of the free spectrahedron of quantum magic squares, but there must be more. It would of course be very interesting to find the remaining extreme points to gain more insight into the structure of quantum magic squares.

Another interesting direction to look into is how we can use quantum magic squares to construct quantum information theoretic structures such as unitary error bases or orthogonal quantum Latin squares and thereby absolutely maximally entangled states.

All in all, we have gained insight into the structures of quantum Latin squares and quantum magic squares but on the way a lot of new questions arose.

9 Appendix

Definition 9.1 (C^*-Algebra)**.** A C^*-algebra is a unital complex algebra $\mathcal{A}$ with an involution * and a complete norm $\|\cdot\|$ satisfying the C^*-identity:

$$\forall T \in \mathcal{A}: \ \|T^*T\| = \|T\|^2$$

The set of hermitian elements and positive elements in $\mathcal{A}$ are give by

$$\mathcal{A}_{her} = \{a \in \mathcal{A} \mid a^* = a\}; \ \mathcal{A}^+ = \{a \in \mathcal{A}_{her} \mid \exists b \in \mathcal{A} : a = b^*b\}$$

Given a Hilbert space $\mathcal{H}$, the set of bounded operators on this space $\mathcal{B}(\mathcal{H})$ forms a C^*-algebra.
If $\mathcal{H}$ is finite dimensional with dimension n, we have $\mathcal{B}(\mathcal{H}) \cong \mathrm{Mat}_n(\mathbb{C})$. In particular, $\mathrm{Mat}_n(\mathbb{C})$ with the operator norm and the conjugate transpose as involution, i.e. $(A_{i,j})^*_{i,j} = (\overline{A_{i,j}}))_{j,i}$, is a C^*-algebra.

Definition 9.2. Let $\mathcal{A}, \mathcal{B}$ be two C^*-algebras. A map $\varphi : \mathcal{A} \to \mathcal{B}$ is called **positive unital $*$-linear map** if

(1) φ is linear in the sense of a map between two $\mathbb{C}$-vector spaces.

(2) φ preserves the involution, i.e. for any $a \in \mathcal{A} : \varphi(a^*) = \varphi(a)^*$

(3) φ maps the one element (in the algebra structure) of $\mathcal{A}$ to the one element of $\mathcal{B}$.

(4) φ preserves positivity, i.e. $\varphi(\mathcal{A}^+) \subseteq \mathcal{B}^+$

A matrix $U \in \mathrm{Mat}_n(\mathbb{C})$ is called unitary, if $UU^* = UU^* = \mathrm{I}$

9.1 Convex Cones and their Properties

Definition 9.3 (Convex cone)**.** A subset C of a vector space V over $\mathbb{R}$ or $\mathbb{C}$ is called a convex cone, if $\forall a, b \in C$ and $\forall \alpha, \beta \in \mathbb{R}_{\geq 0}$ it holds that

$$\alpha a + \beta b \in C.$$

Definition 9.4 (Salient Convex Cone)**.** A convex cone C is said to be salient, if and only if $C \cap -C = \{0\}$.

A non-salient convex cone always contains no less than one linear subset of dimension at least one. A salient cone is always peaked at 0.
For example the half plain $C_1 = \{(x, y) \in \mathbb{R}^2 | x \geq 0\}$ is non-salient because it contains the linear subset $\{(0, y)|y \in \mathbb{R}\}$ which is also contained in $-C_1 = \{(x, y) \in \mathbb{R}^2 | x \leq 0\}$. Conversely, the positive orthant

$$C_2 = \{a(1, 0) + b(0, 1)| \ a, b \in \mathbb{R}_{\geq 0}\}$$

is salient as no vector with a negative component is in the cone. Both cones are depicted in Figure 2.

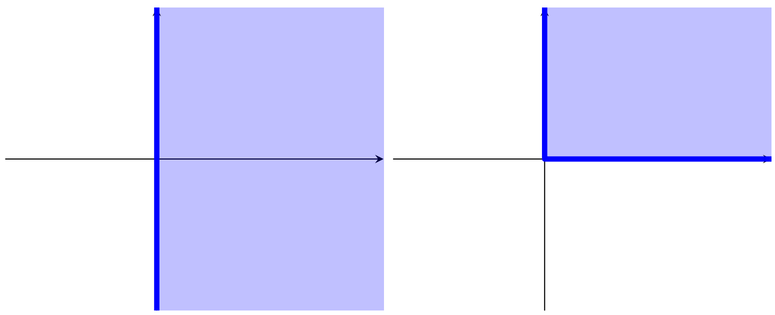

Figure 2: The half plain, non-salient, and the positive orthant, salient

Definition 9.5 (Polyhedral Cone)**.** A cone is called **polyhedral** if it is of the form

$$\{a \in \mathbb{R}^n \mid v_1^* a \geq 0, \ldots, v_d^* a \geq 0\}$$

for some $v_1, \ldots, v_d \in \mathbb{R}^n$.

Note: Every polyhedral cone is a spectrahedral cone.

Definition 9.6 (Simplex cone)**.** A cone $C \subseteq \mathbb{R}^d$ is said to be a simplex cone if it is generated by d linear independent elements, i.e.
there exist $c_1, ..., c_d \in C$ linear independent, such that

$$C = \left\{ \sum_{i=1}^{d} \lambda_i c_i | \ \lambda_i \in \mathbb{R}_{\geq 0} \right\}$$

Definition 9.7 (Extreme Rays)**.** [4] Given a polyhedral cone $C \subseteq \mathbb{R}^n$ and $v \in C$. Then $co(v) = \{\lambda v \mid \lambda \geq 0\}$ is called the **ray** spanned by v.
A ray $R \subseteq C$ is called an **extreme ray** if for any $v \in R$ we have for any $u, w \in C$ that $v = \frac{u+w}{2} \Rightarrow u, w \in R$.

Definition 9.8 (Faces and Facets)**.** Let $K \subseteq \mathbb{R}^n$ be a closed convex set. $F \subset K$ is called a **face** of K if it is convex and whenever, for $v, w \in K, \lambda \in (0,1)$, we have $\lambda v + (1-\lambda)w \in F$ then $v, w \in F$.
A 0 dimensional face is called extreme point. A $n-1$ dimensional face is called facet.
Note: The dimension of a convex set is the dimension of the smallest affine subspace that contains it.

9.2 Minimal and Maximal Operator System: Proofs

Definition 9.9 (Minimal operator system)**.** Let $C \subset \mathbb{R}^m$ be a closed salient convex cone. We define the minimal operator system containing C as $C^{\min} =$

$(C_s^{\min})_{s\geq 1}$ with

$$C_s^{\min} := \left\{ \sum_i c_i \otimes P_i |\ c_i \in C,\ P_i \in \mathrm{PSD}_s \right\}$$

Lemma 9.10. The minimal operator system is minimal in the sense that for all operator systems $(D_s)_{s\geq 1}$ with $D_1 = C$ it follows that $\forall s \in \mathbb{N}:\ C_s^{\min} \subseteq D_s$.

Proof. Let $(D_s)_{s\geq 1}$ be an operator system with $D_1 = C$. Part (2) in the definition of operator systems (2.30) yields that for each matrix $V \in \mathrm{Mat}_{1,s}(\mathbb{C})$ and for every $(c_1, ..., c_m) \in C = D_1$, it holds that $(V^* c_1 V, ..., V^* c_m V) \in D_s$ for an arbitrary $s \in \mathbb{N}$. Because $c_i \in \mathbb{R}$ we get $V^* c_i V = c_i (V^* V) = c_i \otimes (V^* V)$. Now $\forall x \in \mathbb{C}^s:\ x^* V^* V x = (Vx)^*(Vx) = \langle Vx, Vx\rangle \geq 0$. Therefore $V^* V \in \mathrm{PSD}_s$.
On the other hand each positive semi-definite matrix A can be factorized, such that $A = \sum_i v_i v_i^*$ for some column vectors $v_i \in \mathbb{C}^s$. Then we can write $A = \sum_i V_i^* V_i$ with $V_i = v_i^*$.
Therefore an element $\sum_i c_i \otimes P_i \in C_s^{\min}$ can be written as

$$\begin{aligned} \sum_i c_i \otimes P_i &= \sum_i c_i \otimes \sum_j V_{i,j}^* V_{i,j} \\ &= \sum_i \sum_j V_{i,j}^* c_i V_{i,j} \in D_s \end{aligned} \tag{1}$$

That (1) holds follows from the fact that $V_{i,j} \in \mathrm{Mat}_{1,s}$ and from using part 2) in the definition of operator systems. $\square$

Definition 9.11 (Maximal operator system)**.** Let $C \subset \mathbb{R}^m$ be a closed salient convex cone. Then the maximal operator system containing C is given by:

$$C_s^{\max} = \{(B_1, ..., B_m) \in \mathrm{Her}_s(\mathbb{C})^m |\ \forall v \in \mathbb{C}^s\ (v^* B_1 v, ..., v^* B_m) \in C\}.$$

We write $C^{\max}$ as short form for the family $(C_s^{\max})_{s\geq 1}$

Lemma 9.12. $C^{\max}$ is the maximal operator system, where maximal in this context means that for any operator system $(D_r)_{r\geq 1}$ with $D_1 \subseteq C$ it holds that $D_s \subseteq C_s^{\max}$.

Proof. Let $(D_r)_{r\geq 1}$ be an operator system with $D_1 \subseteq C$. If $(B_1, ..., B_m) \in D_s$ then Definition 2.30 2) shows us that $\forall v \in \mathbb{C}^s:\ (v^* B_1 v, ..., v^* B_m v) \in D_1 \subseteq C$. Therefore $(B_1, ..., B_m) \in C_s^{\max}$. $\square$

9.3 Free Spectrahedron

Definition 9.13 (Spectrahedron)**.** The spectrahedron generated by the matrices
$A_1, ..., A_m \in \mathrm{Her}_s(\mathbb{C})$ is given by

$$S(A_1, .., A_m) := \left\{ (b_1, ..., b_m) \in \mathbb{R}^m \mid \sum_{i=1}^m b_i A_i \geq 0 \right\}.$$

Generalizing the spectrahedron for the non-commutative case leads to the definition of the free spectrahedron.

Definition 9.14 (Free spectrahedron)**.** The r-level of the free spectrahedron defined by $A_1, ..., A_m \in \mathrm{Her}_s(\mathbb{C})$ with $r \in \mathbb{N}$ is given by

$$FS_r(A_1, ..., A_m) := \left\{ (B_1, ..., B_m) \in \mathrm{Her}_r(\mathbb{C})^m | \sum_{i=1}^{m} A_i \otimes B_i \geq 0 \right\}$$

The free spectrahedron defined by $A_1, ..., A_m$ is the collection of the above:

$$FS(A_1, ..., A_m) := (FS_r(A_1, ..., A_m))_{r \in \mathbb{N}}$$

Note that the 1-level of the free spectrahedron equals the spectrahedron.

Lemma 9.15. For $r \in \mathbb{N}$ and linear independent $A_1, ..., A_m \in \mathrm{Her}_s(\mathbb{C})$, the r-level of the free spectrahedron defined by $A_1, ..., A_m$ is a closed salient convex cone.

Proof. Short calculation shows that $FS_r(A_1, ..., A_m)$ is a convex cone.
Let $(B_1, ..., B_m) \in FS_r(A_1, ..., A_m) \backslash \{0\}$, then $\sum_{i=1}^{m} A_i \otimes B_i \geq 0$. Due to the linearity of the tensor product it follows that $\sum_{i=1}^{m} A_i \otimes (-B_i) = -\sum_{i=1}^{m} A_i \otimes B_i$ is negative semidefinite. If $\sum_{i=1}^{m} A_i \otimes B_i = 0$ the linear independence of the A_i induces that $B_1 = ... = B_m = 0$ which contradicts our choice of the B_i. Therefore $-(B_1, ..., B_m) \notin FS_r(A_1, ..., A_m)$.
It is known that the r-level of the free spectrahedron is closed, as the property of being positive semidefinite is a closed condition. For each vector v, $v^* A v \geq 0$ is already a closed condition. □

9.4 Notation

In this section, we give a quick overview over the standard notation used in this work.

$\mathrm{Mat}_n(\mathbb{C})$ denotes the $\mathbb{C}^*$-algebra of complex $n \times n$ matrices with the usual matrix addition, multiplication and the involution given by $\left((A_{i,j})_{i,j=1}^n\right)^* := (\overline{A_{j,i}})_{i,j=1}^n$.

$\mathrm{Her}_n(\mathbb{C})$ denotes the hermitian elements in $\mathrm{Mat}_n(\mathbb{C})$, i.e. those matrices $A \in \mathrm{Mat}_n(\mathbb{C})$ for which $A^* = A$.

PSD_n is the set of positive semi-definite matrices of size n, i.e. the positive elements in the C^*-algebra $\mathrm{Mat}_n(\mathbb{C})$.

$$\delta_{i,j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{else} \end{cases}$$

denotes the Kronecker delta.

$\mathrm{I}_n = (\delta_{i,j})_{i,j=1}^n$ is the $n \times n$ identity matrix, the one-element in $\mathrm{Mat}_n(\mathbb{C})$.

$\mathbb{N} = \{1, 2, 3, \ldots\}$ denotes the natural numbers without zero.

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